(51) International Patent Classification 6 : C12N 9/02 // (C12N 9/02, C12R 1:645)	**A1**	(11) International Publication Number: **WO 98/27198**
		(43) International Publication Date: 25 June 1998 (25.06.98)

(21) International Application Number: PCT/DK97/00571

(22) International Filing Date: 16 December 1997 (16.12.97)

(30) Priority Data:
1449/96   19 December 1996 (19.12.96)   DK
1021/97   8 September 1997 (08.09.97)   DK

(71) Applicant: NOVO NORDISK A/S [DK/DK]; Novo Allé, DK–2880 Bagsvaerd (DK).

(72) Inventors: PEDERSEN, Anders, Hjelholt; Nybro Vaenge 58, DK–2800 Lyngby (DK). SVENDSEN, Allan; Bakkeledet 28, DK–3460 Birkerød (DK). SCHNEIDER, Palle; Rydtoften 43, DK–2750 Ballerup (DK). RASMUSSEN, Grethe; Brudedalen 1, DK–3520 Farum (DK). CHERRY, Joel, R.; C.V.E. Knuthsvej 9, DK–2100 Hellerup (DK).

(74) Common Representative: NOVO NORDISK A/S; Corporate Patents, Novo Allé, DK–2880 Bagsværd (DK).

(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

Published
With international search report.

(54) Title: LACCASE MUTANTS

(57) Abstract

The present invention relates to a method of designing laccase mutants with improved stability properties, which method is based on the hitherto unknown three–dimensional structure of *Coprinus cinereus* laccase.

FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AL	Albania	ES	Spain	LS	Lesotho	SI	Slovenia
AM	Armenia	FI	Finland	LT	Lithuania	SK	Slovakia
AT	Austria	FR	France	LU	Luxembourg	SN	Senegal
AU	Australia	GA	Gabon	LV	Latvia	SZ	Swaziland
AZ	Azerbaijan	GB	United Kingdom	MC	Monaco	TD	Chad
BA	Bosnia and Herzegovina	GE	Georgia	MD	Republic of Moldova	TG	Togo
BB	Barbados	GH	Ghana	MG	Madagascar	TJ	Tajikistan
BE	Belgium	GN	Guinea	MK	The former Yugoslav	TM	Turkmenistan
BF	Burkina Faso	GR	Greece		Republic of Macedonia	TR	Turkey
BG	Bulgaria	HU	Hungary	ML	Mali	TT	Trinidad and Tobago
BJ	Benin	IE	Ireland	MN	Mongolia	UA	Ukraine
BR	Brazil	IL	Israel	MR	Mauritania	UG	Uganda
BY	Belarus	IS	Iceland	MW	Malawi	US	United States of America
CA	Canada	IT	Italy	MX	Mexico	UZ	Uzbekistan
CF	Central African Republic	JP	Japan	NE	Niger	VN	Viet Nam
CG	Congo	KE	Kenya	NL	Netherlands	YU	Yugoslavia
CH	Switzerland	KG	Kyrgyzstan	NO	Norway	ZW	Zimbabwe
CI	Côte d'Ivoire	KP	Democratic People's	NZ	New Zealand		
CM	Cameroon		Republic of Korea	PL	Poland		
CN	China	KR	Republic of Korea	PT	Portugal		
CU	Cuba	KZ	Kazakstan	RO	Romania		
CZ	Czech Republic	LC	Saint Lucia	RU	Russian Federation		
DE	Germany	LI	Liechtenstein	SD	Sudan		
DK	Denmark	LK	Sri Lanka	SE	Sweden		
EE	Estonia	LR	Liberia	SG	Singapore		

LACCASE MUTANTS

FIELD OF THE INVENTION

5   The present invention relates to a method of designing
laccase mutants with improved stability properties, which method
is based on the hitherto unknown three-dimensional structure of
laccases.

10 ## BACKGROUND OF THE INVENTION

Laccase is a polyphenol oxidase (EC 1.10.3.2) which catalyses
the oxidation of a variety of inorganic and aromatic compounds,
particularly phenols, with the concomitant reduction of molecular
15 oxygen to water.

Laccase belongs to a family of blue copper-containing
oxidases which includes ascorbate oxidase and the mammalian
plasma protein ceruloplasmin. All these enzymes are multi-copper-
containing proteins.

20   Because laccases are able to catalyze the oxidation of a
variety of inorganic and aromatic compounds, laccases have been
suggested in many potential industrial applications such as
lignin modification, paper strengthening, dye transfer inhibition
in detergents, phenol polymerization, hair colouring, and waste
25 water treatment. A major problem with the use of laccases are
their poor storage stability at temperatures above room
temperature, especially at 40°C.

In Example 1 of the present application we have tested the
stability of various laccases at 40°C, and it can be seen that
30 after 2 weeks of storage the laccase activity is down to less
than 50% of the initial value, and at low pH the laccase activity
after 2 weeks is zero. For many purposes such a decrease is
unacceptable, so it is the purpose of the present invention to
create laccase variants with improved stability by using the
35 information of a three-dimensional structure of a *Coprinus
cinereus* laccase. No three-dimensional structural information has
been available for a laccase before.

BRIEF DISCLOSURE OF THE INVENTION

The three-dimensional structure of a laccase has now been elucidated. On the basis of an analysis of said structure it is possible to identify structural parts or specific amino acid residues which from structural or functional considerations appear to be important for the stability of a laccase.

Furthermore, when comparing the three-dimensional structure of the Coprinus laccase structure with known amino acid sequences of various laccases, it has been found that some similarities exist between the sequences. The present invention is based on these findings.

Accordingly, in a first aspect the invention relates to a method of constructing a variant of a parent Coprinus laccase, which variant has laccase activity and improved stability as compared to said parent laccase, which method comprises

i) analysing the three-dimensional structure of the parent Coprinus laccase to identify at least one amino acid residue or at least one structural part of the Coprinus laccase structure, which amino acid residue or structural part is believed to be of relevance for altering the stability of the parent Coprinus laccase (as evaluated on the basis of structural or functional considerations),

ii) constructing a Coprinus laccase variant, which as compared to the parent Coprinus laccase, has been modified in the amino acid residue or structural part identified in i) so as to alter the stability, and, optionally,

iii) testing the resulting Coprinus laccase variant with respect to stability.

In a second aspect the present invention relates to a method of constructing a variant of a parent Coprinus-like laccase, which variant has laccase activity and improved stability as compared to said parent laccase, which method comprises
i) comparing the three-dimensional amino acid structure of the

Coprinus laccase with an amino acid sequence of a *Coprinus*-like
laccase,

ii) identifying a part of the *Coprinus*-like laccase amino acid
5 sequence which is different from the *Coprinus* laccase amino acid
sequence and which from structural or functional considerations
is contemplated to be responsible for differences in the
stability of the *Coprinus* and *Coprinus*-like laccase,

10 iii) modifying the part of the *Coprinus*-like laccase identified
in ii) whereby a *Coprinus*-like laccase variant is obtained, which
has an improved stability as compared to the parent *Coprinus*-like·
laccase, and optionally,

15 iv) testing the resulting *Coprinus*-like laccase variant with
respect to stability.

In still further aspects the invention relates to variants of
a *Coprinus* laccase and of *Coprinus*-like laccases, DNA encoding
20 such variants and methods of preparing the variants. Finally, the
invention relates to the use of the variants for various
industrial purposes.

DETAILED DISCLOSURE OF THE INVENTION
25

The *Coprinus*-like laccases

A number of laccases produced by different fungi are
homologous on the amino acid level. For instance, when using the
homology percent obtained from UWGCG program using the GAP
30 program with the default parameters (penalties: gap weight=3.0,
length weight=0.1; WISCONSIN PACKAGE Version 8.1-UNIX, August
1995, Genetics Computer Group, 575 Science Drive, Madison,
Wisconsin, USA 53711) the following homology was found:
Coprinus cinereus laccase comprising the amino acid sequence
35 shown in SEQ ID No. 1: 100%;
Polyporus pinsitus (I) laccase comprising the amino acid sequence

shown in SEQ ID No. 2: 74.4%;

Polyporus pinsitus (II) laccase comprising the amino acid sequence shown in SEQ ID No. 3: 73.8%;

Phlebia radiata laccase comprising the amino acid sequence shown in SEQ ID No. 4: 69.9% ;

Rhizoctonia solani (I) laccase comprising the amino acid sequence shown in SEQ ID No. 5: 64.8%;

Rhizoctonia solani (II) laccase comprising the amino acid sequence shown in SEQ ID No. 6: 63.0%;

Rhizoctonia solani (III) laccase comprising the amino acid sequence shown in SEQ ID No. 7: 61.0%;

Rhizoctonia solani (IV) laccase comprising the amino acid sequence shown in SEQ ID No. 8: 59.7%;

Scytalidium thermophilum laccase comprising the amino acid sequence shown in SEQ ID No. 9: 57.4%;

Myceliophthora thermophila laccase comprising the amino acid sequence shown in SEQ ID No. 10: 56.5%.

Because of the homology found between the above mentioned laccases, they are considered to belong to the same class of laccases, namely the class of "*Coprinus*-like laccases".

Accordingly, in the present context, the term "*Coprinus*-like laccase" is intended to indicate a laccase which, on the amino acid level, displays a homology of at least 50% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 55% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 60% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 65% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 70% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 75% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 80% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 85% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or at least 90% and less than 100% to the *Coprinus cinereus* laccase SEQ ID NO 1, or

at least 95% and less than 100% to the *Coprinus cinereus* laccase
SEQ ID NO 1.

In the present context, "derived from" is intended not only
to indicate a laccase produced or producible by a strain of the
5 organism in question, but also a laccase encoded by a DNA
sequence isolated from such strain and produced in a host or-
ganism containing said DNA sequence. Finally, the term is
intended to indicate a laccase which is encoded by a DNA sequence
of synthetic and/or cDNA origin and which has the identifying
10 characteristics of the laccase in question.

The three-dimensional *Coprinus* laccase structure

The *Coprinus* laccase which was used to elucidate the three-
dimensional structure forming the basis for the present invention
15 consists of the 539 amino acids derived from *Coprinus cinereus*
laccase IFO 8371 as disclosed in sequence ID No. 1.

The obtained three-dimensional structure is believed to be
representative for the structure of any *Coprinus*-like laccase.

The structure of the laccase was solved in accordance with
20 the principle for X-ray crystallographic methods given in "X-Ray
Structure Determination", Stout, G.K. and Jensen, L.H., John
Wiley & Sons, inc. NY, 1989. The structural coordinates for the
solved crystal structure of the laccase at 2.2 Å resolution using
the isomorphous replacement method are given in a standard PDB
25 format (Brookhaven Protein Data Base) in Appendix 1. It is to be
understood that Appendix 1 forms part of the present application.

In Appendix 1 the amino acid residues of the enzyme are
identified by three-letter amino acid code (capitalized letters).

The laccase structure is made up of three plastocyanin-like
30 domains. These three domains all have a similar beta-barrel fold.

3 copper atoms were observed in the three-dimensional
structure:

The so-called type 1 copper ion is coordinated by two
histidines and one cysteine.
35 The so-called type 2 copper of the trinuclear centre is
missing in the structure disclosed in the present application.

The so-called type 3 copper consists of two type 3 copper

atoms (pair of copper atoms) bound to a total of 6 histidine ligands.

When comparing the amino acid sequence of the crystallized three-dimensional structure with *Coprinus cinereus* amino acid
5 sequence ID No. 1 the following four differences are observed:

18 amino acids are missing from the N-terminal of the crystallized protein;

17 amino acids are missing from the C-terminal of the crystallized protein;

10 Q19 in sequence ID No. 1 is an A1 in the crystallized protein; and

Q243 in sequence ID No. 1 is an E225 in the crystallized protein.

Generality of structure

15 Because of the homology between the *Coprinus* laccase and the various *Coprinus*-like laccases, the solved structure defined by the coordinates of Appendix 1 is believed to be representative for the structure of all *Coprinus*-like laccases. A model structure of *Coprinus*-like laccases may be built on the basis of
20 the coordinates given in Appendix 1 adapted to the laccase in question by use of an alignment between the respective amino acid sequences.

The above identified structurally characteristic parts of the *Coprinus* laccase structure may be identified in other *Coprinus*-
25 like laccases on the basis of a model (or solved) structure of the relevant *Coprinus*-like laccase or simply on the basis of an alignment between the amino acid sequence of the *Coprinus*-like laccase in question with that of the *Coprinus* laccase used herein for identifying the amino acid residues of the respective
30 structural elements.

Furthermore, in connection with *Coprinus* laccase variants of the invention, which are defined by modification of specific amino acid residues of the parent *Coprinus* laccase, it will be understood that variants of *Coprinus*-like laccases modified in an
35 equivalent position (as determined from the best possible amino acid sequence alignment between the respective sequences) are

intended to be covered as well.

Methods of the invention for design of novel laccase variants

The analysis or comparison performed in step i) of the
5 methods of the invention may be performed by use of any suitable
computer programme capable of analysing and/or comparing amino
acid sequences.

The structural part which is identified in step i) of the
methods of the invention may be composed of one amino acid
10 residue. However, normally the structural part comprises more
than one amino acid residue, typically constituting one of the
above mentioned parts of the *Coprinus* structure such as one of
the copper centres.

According to the invention useful laccase variants may be
15 modified in one or more amino acid residues present within 15 Å
from any copper ion, preferably variants which are modified
within 10 Å from any copper ion, in particular variants which are
modified within 5 Å from any copper ion.

Determination of residues within 5Å, 10Å and 15Å from the
20 copper ions in the three-dimensional structure: The coordinates
from the appendix are read into INSIGHT program provided by
BIOSYM technologies. The spatial coordinates are presented
showing the bonds between the atoms. The copper atoms are
presented as well as the water atoms. The program package
25 contains a part which can be used for creating subsets. This part
is used for creating a 5Å, 10Å and 15Å subset around all Cu-ions
present in the structure (the command ZONE is used).   The
found subsets contain all residues having an atom within 5, 10
and 15Å from any of the Cu-ions present in the structure. All
30 residues having an atom within this subset are compiled and
written out by the LIST MOLECULE command.

The amino acid residues found in this way within a distance
of 15 Å from a copper ion in the *Coprinus cinereus* laccase are
the following (SEQ ID No 1 numbering):
35 M27, V46, G51, P52, I54, L64, L76, T79, S80, I81, H82, W83, H84,
G85, L86, F87, Q88, R89, T91, N92, W93, A94, D95, G96, A97, D98,
G99, V100, N101, Q102, C103, P104, Y113, F115, H120, G122, T123,
F124, W125, Y126, H127, S128, H129, F130, G131, T132, Q133, Y134,

C135, D136, G137, L138, R139, G140, P141, M142, V143, I144, I164,
T165, L166, A167, D168, H170, G179, A180, A181, Q182, P183, L217,
I218, S219, L220, S221, C222, D223, P224, N225, W226, E239, V240,
D241, G242, Q243, Q254, I255, F256, T257, G258, Q259, R260, Y261,
5 N281, K282, F349, Q350, L351, G352, F353, S354, G356, R357, F358,
T359, I360, N361, T363, A364, Y365, E366, S367, P368, P371, T372,
L373, P388, S391, V392, L403, V404, V405, P406, A407, G408, V409,
L410, G411, G412, P413, H414, P415, F416, H417, L418, H419, G420,
H421, A422, F423, A429, K441, R442, D443, V444, V445, S446, L447,
10 G448, V449, T450, D452, V454, I456, F458, N462, G464, P465, W466,
F467, F468, H469, C470, H471, I472, E473, F474, H475, L476, M477,
N478, G479, L480, A481, I482, V483, F484, A485, E486.

The amino acid residues found within a distance of 10 Å from
a copper ion in the *Coprinus cinereus* laccase (SEQ ID No 1) are
15 the following:

S80, I81, H82, W83, H84, G85, L86, D95, G96, A97, D98, V100,
N101, F124, W125, Y126, H127, S128, H129, F130, G131, Y134, L138,
R139, G140,, I218, S219, L220, S221, C222, D223, P224, D241,
F256, T257, G258, Q259, R260, K282, L351, G352, F353, F358, T359,
20 V405, V409, L410, G411, G412, P413, H414, P415, F416, H417, L418,
H419, G420, D443, V444, V445, S446, L447, G448, V454, I456, F458,
W466, F467, F468, H469, C470, H471, I472, E473, F474, H475, L476,
M477, N478, G479, L480, A481, I482.

The amino acid residues found within a distance of 5 Å from a
25 copper ion in the *Coprinus cinereus* laccase (SEQ ID No 1) are the
following:

H82, H84, W125, H127, H129, G411, H414, P415, H417, H419, F467,
H469, C470, H471, I472, H475, L480.

The 15Å/10Å/5Å regions can be found in other laccases by
30 comparison of the modelled structures or by taking the sequence
homology numbers.

Modifications

The modification of an amino acid residue or structural part
35 is typically accomplished by suitable modifications of a DNA
sequence encoding the parent enzyme in question. The term
"modified" as used in the methods according to the invention is
intended to have the following meaning: When used in relation to

an amino acid residue the term is intended to mean replacement of the amino acid residue in question with another amino acid residue. When used in relation to a structural part, the term is intended to mean: replacement of one or more amino acid residues
5 of said structural part with other amino acid residues, or addition of one or more amino acid residues to said part, or deletion of one or more amino acid residues of said structural part.

The construction of the variant of interest is accomplished
10 by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth. This is described in detail further below.
15

Variants with altered stability

It is contemplated that it is possible to improve the stability of a parent *Coprinus* laccase or a parent *Coprinus*-like laccase, wherein said variant is the result of a mutation, i.e.
20 one or more amino acid residues having been deleted from, replaced or added to the parent laccase, the stability test performed as described below.

Preferred positions for mutations are the following:

MtL:	StL:	CcL:	PpL1:	PpL2:	PrL:	RsL4:	RsL1:	RsL2:	RsL3:
M433	M483	-	-	-	-	-	-	-	-
W373	W422	-	-	-	-	W411	W411	W439	-
W136	W181	W125	W107	W107	W128	W125	W125	W125	W126
Y145	Y190	Y134	Y116	Y116	Y137	Y134	Y134	Y134	Y135
M480	M530	-	-	-	-	-	-	-	-
Y137	Y182	Y126	Y108	Y108	Y129	Y126	Y126	Y126	Y127
Y176	Y221	Y170	Y152	Y152	Y137	Y170	Y169	Y170	Y171
M254	M300	-	-	-	-	-	-	-	-
-	-	M75	M57	M57	M78	M75	M75	M75	M76
-	-	M477	-						
			M328						
-	M313	-	-						

W507,

wherein

CcL: *Coprinus cinereus* laccase comprising the amino acid sequence
shown in SEQ ID No. 1;

5 PpL1: *Polyporus pinsitus (I)* laccase comprising the amino acid
sequence shown in SEQ ID No. 2;

PpL2: *Polyporus pinsitus (II)* laccase comprising the amino acid
sequence shown in SEQ ID No. 3;

PrL: *Phlebia radiata* laccase comprising the amino acid sequence
10 shown in SEQ ID No. 4;

RsL3: *Rhizoctonia solani (I)* laccase comprising the amino acid
sequence shown in SEQ ID No. 5;

RsL2: *Rhizoctonia solani (II)* laccase comprising the amino acid
sequence shown in SEQ ID No. 6;

15 RsL4: *Rhizoctonia solani (III)* laccase comprising the amino acid
sequence shown in SEQ ID No. 7;

RsL1: *Rhizoctonia solani (IV)* laccase comprising the amino acid
sequence shown in SEQ ID No. 8;

StL: *Scytalidium thermophilum* laccase comprising the amino acid
20 sequence shown in SEQ ID No. 9; and

MtL: *Myceliophthora thermophila* laccase comprising the amino acid
sequence shown in SEQ ID No. 10.

The above shown rows have homologous positions. (-) or ( ) =
25 not present in this laccase.

The following variants are preferred:

A variant of a parent *Coprinus* laccase, which comprises one
30 or more of the following substitutions in SEQ ID No. 1:

W125 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;

Y134 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y126 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y170 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

35 M75 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;

M477 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Coprinus* laccase, which comprises one or more of the following substitutions in SEQ ID No. 1:

5 W125 F, H;

Y134 F;

Y126 F;

Y170 F;

M75   F, V, I, L, Q;

10 M477 F, V, I, L, Q.

A variant of a parent *Polyporus pinsitus (I)* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 2:

15 W107 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;

Y116 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y108 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y152 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

M57   A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;

20 M328 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Polyporus pinsitus (I)* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 2:

25 W107 F, H;

Y116 F;

Y108 F;

Y152 F;

M57   F, V, I, L, Q;

30 M328 F, V, I, L, Q.

A variant of a parent *Polyporus pinsitus (II)* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 3:

35 W107 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;

Y116 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y108 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y152 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
M57 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Polyporus pinsitus (II)*
laccase, which comprises a mutation in a position corresponding
to at least one of the following positions in SEQ ID No. 3:
W107 F, H;
Y116 F;
Y108 F;
Y152 F;
M57 F, V, I, L, Q.

A variant of a parent *Phlebia radiata* laccase, which
comprises a mutation in a position corresponding to at least one
of the following positions in SEQ ID No. 4:
W128 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
Y137 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y129 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y137 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
M78 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Phlebia radiata* laccase,
which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 4:
W128 F, H;
Y137 F;
Y129 F;
Y137 F;
M78 F, V, I, L, Q.

A variant of a parent *Rhizoctonia solani (I)* laccase, which
comprises a mutation in a position corresponding to at least one
of the following positions in SEQ ID No. 5:
W126 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
Y135 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y127 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y171 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

M76 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Rhizoctonia solani (I)*
laccase, which comprises a mutation in a position corresponding
5 to at least one of the following positions in SEQ ID No. 5:
W126 F, H;
Y135 F;
Y127 F;
Y171 F;
10 M76 F, V, I, L, Q.

A variant of a parent *Rhizoctonia solani (II)* laccase, which
comprises a mutation in a position corresponding to at least one
of the following positions in SEQ ID No. 6:
15 W439 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
W125 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
Y134 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y126 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y170 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
20 M75 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

In particular a variant of a parent *Rhizoctonia solani (II)*
laccase, which comprises a mutation in a position corresponding
to at least one of the following positions in SEQ ID No. 6:
25 W439 F, H;
W125 F, H;
Y134 F;
Y126 F;
Y170 F;
30 M75 F, V, I, L, Q.

A variant of a parent *Rhizoctonia solani (III)* laccase,
which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 7:
35 W411 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
W125 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
Y134 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;

Y126 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y170 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
M75 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

5   In particular a variant of a parent *Rhizoctonia solani (III)*
laccase, which comprises a mutation in a position corresponding
to at least one of the following positions in SEQ ID No. 7:
W411 F, H;
W125 F, H;
10 Y134 F;
Y126 F;
Y170 F;
M75 F, V, I, L, Q.

15   A variant of a parent *Rhizoctonia solani (IV)* laccase, which
comprises a mutation in a position corresponding to at least one
of the following positions in SEQ ID No. 8:
W411 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
W125 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
20 Y134 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y126 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
Y170 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
M75 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.

25   In particular a variant of a parent *Rhizoctonia solani (IV)*
laccase, which comprises a mutation in a position corresponding
to at least one of the following positions in SEQ ID No. 8:
W411 F, H;
W125 F, H;
30 Y134 F;
Y126 F;
Y170 F;
M75 F, V, I, L, Q.

35   A variant of a parent *Scytalidium thermophilum* laccase,
which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 9:

```
    M483 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;
    W422 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
    W181 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
    Y190 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
5   M530 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;
    Y182 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
    Y221 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
    M300 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;
    M313 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.
10
```

In particular a variant of a parent *Scytalidium thermophilum* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 9:

```
    M483 F, V, I, L, Q;
15  W422 F, H;
    W181 F, H;
    Y190 F;
    M530 F, V, I, L, Q;
    Y182 F;
20  Y221 F;
    M300 F, V, I, L, Q;
    M313 F, V, I, L, Q.
```

A variant of a parent *Myceliophthora thermophila* laccase,
25 which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 10:

```
    M433 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;
    W373 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
    W136 A, V, L, I, P, F, M, G, S, T, C, Y, N, Q, D, E, K, R, H;
30  Y145 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
    M480 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H;
    Y137 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
    Y176 A, V, L, I, P, F, W, G, S, T, C, M, N, Q, D, E, K, R, H;
    M254 A, V, L, I, P, F, W, G, S, T, C, Y, N, Q, D, E, K, R, H.
35
```

In particular a variant of a parent *Myceliophthora thermophila* laccase, which comprises a mutation in a position

16

corresponding to at least one of the following positions in SEQ
ID No. 10:
M433 F, V, I, L, Q;
W373 F, H;
5 W136 F, H;
Y145 F;
M480 F, V, I, L, Q;
Y137 F;
Y176 F;
10 M254 F, V, I, L, Q.

Methods of preparing laccase variants

    Several methods for introducing mutations into genes are
known in the art. After a brief discussion of the cloning of
15 laccase-encoding DNA sequences, methods for generating mutations
at specific sites within the laccase-encoding sequence will be
discussed.

Cloning a DNA sequence encoding a laccase

    The DNA sequence encoding a parent laccase may be isolated
20 from any cell or microorganism producing the laccase in question,
using various methods well known in the art. First, a genomic DNA
and/or cDNA library should be constructed using chromosomal DNA
or messenger RNA from the organism that produces the laccase to
be studied. Then, if the amino acid sequence of the laccase is
25 known, homologous, labelled oligonucleotide probes may be
synthesized and used to identify laccase-encoding clones from a
genomic library prepared from the organism in question. Alter-
natively, a labelled oligonucleotide probe containing sequences
homologous to a known laccase gene could be used as a probe to
30 identify laccase-encoding clones, using hybridization and washing
conditions of lower stringency.

    A method for identifying laccase-encoding clones involves
inserting cDNA into an expression vector, such as a plasmid,
transforming laccase-negative fungi with the resulting cDNA
35 library, and then plating the transformed fungi onto agar
containing a substrate for laccase, thereby allowing clones
expressing the laccase to be identified.

    Alternatively, the DNA sequence encoding the enzyme may be

prepared synthetically by established standard methods, e.g. the
phosphoroamidite method. In the phosphoroamidite method, oligonu-
cleotides are synthesized, e.g. in an automatic DNA synthesizer,
purified, annealed, ligated and cloned in appropriate vectors.

5   Finally, the DNA sequence may be of mixed genomic and synthe-
tic origin, mixed synthetic and cDNA origin or mixed genomic and
cDNA origin, prepared by ligating fragments of synthetic, genomic
or cDNA origin (as appropriate, the fragments corresponding to
various parts of the entire DNA sequence), in accordance with
10 standard techniques. The DNA sequence may also be prepared by
polymerase chain reaction (PCR) using specific primers.

Site-directed mutagenesis

       Once a laccase-encoding DNA sequence has been isolated, and
15 desirable sites for mutation identified, mutations may be intro-
duced using synthetic oligonucleotides. These oligonucleotides
contain nucleotide sequences flanking the desired mutation sites;
mutant nucleotides are inserted during oligonucleotide synthesis.
In a specific method, a single-stranded gap of DNA, bridging the
20 laccase-encoding sequence, is created in a vector carrying the
laccase gene. Then the synthetic nucleotide, bearing the desired
mutation, is annealed to a homologous portion of the single-
stranded DNA. The remaining gap is then filled in with T7 DNA
polymerase and the construct is ligated using T4 ligase. A
25 specific example of this method is described in Morinaga et al.
(1984). US 4,760,025 discloses the introduction of oligonucleoti-
des encoding multiple mutations by performing minor alterations
of the cassette. However, an even greater variety of mutations
can be introduced at any one time by the Morinaga method, because
30 a multitude of oligonucleotides, of various lengths, can be
introduced.

       Another method of introducing mutations into laccase-encoding
DNA sequences is described in Nelson and Long (1989). It involves
the 3-step generation of a PCR fragment containing the desired
35 mutation introduced by using a chemically synthesized DNA strand
as one of the primers in the PCR reactions. From the PCR-gener-
ated fragment, a DNA fragment carrying the mutation may be
isolated by cleavage with restriction endonucleases and

reinserted into an expression plasmid.

Random mutagenesis

The random mutagenesis of a DNA sequence encoding a parent
5 laccase may conveniently be performed by use of any method known
in the art.

For instance, the random mutagenesis may be performed by use
of a suitable physical or chemical mutagenizing agent, by use of
a suitable oligonucleotide, or by subjecting the DNA sequence to
10 PCR generated mutagenesis. Furthermore, the random mutagenesis
may be performed by use of any combination of these mutagenizing
agents.

The mutagenizing agent may, e.g., be one which induces tran-
sitions, transversions, inversions, scrambling, deletions, and/or
15 insertions.

Examples of a physical or chemical mutagenizing agent
suitable for the present purpose include ultraviolet (UV) ir-
radiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine
(MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane
20 sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide
analogues.

When such agents are used, the mutagenesis is typically per-
formed by incubating the DNA sequence encoding the parent enzyme
to be mutagenized in the presence of the mutagenizing agent of
25 choice under suitable conditions for the mutagenesis to take
place, and selecting for mutated DNA having the desired
properties.

When the mutagenesis is performed by the use of an oligo-
nucleotide, the oligonucleotide may be doped or spiked with the
30 three non-parent nucleotides during the synthesis of the
oligonucleotide at the positions which are to be changed. The
doping or spiking may be done so that codons for unwanted amino
acids are avoided. The doped or spiked oligonucleotide can be
incorporated into the DNA encoding the laccase enzyme by any
35 published technique, using e.g. PCR, LCR or any DNA polymerase
and ligase.

When PCR-generated mutagenesis is used, either a chemically
treated or non-treated gene encoding a parent laccase enzyme is

subjected to PCR under conditions that increase the mis-
incorporation of nucleotides (Deshler 1992; Leung et al.,
Technique, Vol.1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., Molec. Gen.
5 Genet., 133, 1974, pp. 179-191), *S. cereviseae* or any other
microbial organism may be used for the random mutagenesis of the
DNA encoding the laccase enzyme by e.g. transforming a plasmid
containing the parent enzyme into the mutator strain, growing the
mutator strain with the plasmid and isolating the mutated plasmid
10 from the mutator strain. The mutated plasmid may subsequently be
transformed into the expression organism.

The DNA sequence to be mutagenized may conveniently be
present in a genomic or cDNA library prepared from an organism
expressing the parent laccase enzyme. Alternatively, the DNA se-
15 quence may be present on a suitable vector such as a plasmid or a
bacteriophage, which as such may be incubated with or otherwise
exposed to the mutagenizing agent. The DNA to be mutagenized may
also be present in a host cell either by being integrated in the
genome of said cell or by being present on a vector harboured in
20 the cell. Finally, the DNA to be mutagenized may be in isolated
form. It will be understood that the DNA sequence to be subjected
to random mutagenesis is preferably a cDNA or a genomic DNA
sequence.

In some cases it may be convenient to amplify the mutated DNA
25 sequence prior to the expression step or the screening step being
performed. Such amplification may be performed in accordance with
methods known in the art, the presently preferred method being
PCR-generated amplification using oligonucleotide primers
prepared on the basis of the DNA or amino acid sequence of the
30 parent enzyme.

Subsequent to the incubation with or exposure to the mutage-
nizing agent, the mutated DNA is expressed by culturing a
suitable host cell carrying the DNA sequence under conditions
allowing expression to take place. The host cell used for this
35 purpose may be one which has been transformed with the mutated
DNA sequence, optionally present on a vector, or one which was
carried the DNA sequence encoding the parent enzyme during the
mutagenesis treatment. Examples of suitable host cells are fungal

hosts such as *Aspergillus niger* or *Aspergillus oryzae.*

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA
5 sequence.

Localized random mutagenesis
    The random mutagenesis may advantageously be localized to a part of the parent laccase in question. This may, e.g., be
10 advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has
15 been elucidated and related to the function of the enzyme.
    The localized random mutagenesis is conveniently performed by use of PCR-generated mutagenesis techniques as described above or any other suitable technique known in the art.
    Alternatively, the DNA sequence encoding the part of the DNA
20 sequence to be modified may be isolated, e.g. by being inserted into a suitable vector, and said part may subsequently be subjected to mutagenesis by use of any of the mutagenesis methods discussed above.
    With respect to the screening step in the above-mentioned
25 method of the invention, this may conveniently be performed by use of aa filter assay based on the following principle:
    A microorganism capable of expressing the mutated laccase enzyme of interest is incubated on a suitable medium and under suitable conditions for the enzyme to be secreted, the medium
30 being provided with a double filter comprising a first protein-binding filter and on top of that a second filter exhibiting a low protein binding capability. The microorganism is located on the second filter. Subsequent to the incubation, the first filter comprising enzymes secreted from the microorganisms is separated
35 from the second filter comprising the microorganisms. The first filter is subjected to screening for the desired enzymatic activity and the corresponding microbial colonies present on the second filter are identified.

The filter used for binding the enzymatic activity may be any protein binding filter e.g. nylon or nitrocellulose. The top filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins e.g.
5 cellulose acetate or Durapore™. The filter may be pretreated with any of the conditions to be used for screening or may be treated during the detection of enzymatic activity.

The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any
10 other known technique for detection of enzymatic activity.

The detecting compound may be immobilized by any immobilizing agent, e.g., agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents.

15 <u>Testing of variants of the invention</u>

The storage stability of *Coprinus* variants or *Coprinus*-like variants should be investigated at 40°C for 2 weeks at pH 5, 8 and 9.3, respectively. The stability of the parent laccase and the variants may be tested both in a liquid buffer formulation
20 and in a lyophilized form.

According to the invention the residual activity of the variants following two weeks of incubation are then compared to the residual activity of the parent laccase, and variants with an improved stability at either pH 5, 8 or 9.3 are selected.
25

<u>Laccase activity</u>

In the context of this invention, the laccase activity was measured using 10-(2-hydroxyethyl)-phenoxazine (HEPO) as substrate for the various laccases. HEPO was synthesized using
30 the same procedure as described for 10-(2-hydroxyethyl)-phenothiazine, (G. Cauquil in Bulletin de la Society Chemique de France, 1960, p. 1049). In the presence of oxygen laccases (E.C. 1.10.3.2) oxidize HEPO to a HEPO radical that can be monitored photometrically at 528 nm.

35 The *Coprinus cinereus* laccase was measured using 0.4 mM HEPO in 50 mM sodium acetate, pH 5.0, 0.05% TWEEN-20 at 30°C. The absorbance at 528 nm was followed for 200 s and the rate calculated from the linear part of the progress curve.

The *Myceliophthora thermophila* laccase was measured using
0.4 mM HEPO in 25 mM Tris-HCl, pH 7.5, 0.05% Tween-20 at 30 °C.
The absorbance at 528 nm was followed for 200 s and the rate
calculated from the linear part of the progress curve.

5   The *Polyporus pinsitus* laccase was measured using 0.4 mM
HEPO in 50 mM MES-NaOH, pH 5.5. The absorbance at 528 nm was
followed for 200 s and the rate calculated from the linear part
of the progress curve.

10 <u>Expression of laccase variants</u>

       According to the invention, a DNA sequence encoding the
variant produced by methods described above, or by any alterna-
tive methods known in the art, can be expressed, in enzyme form,
using an expression vector which typically includes control
15 sequences encoding a promoter, operator, ribosome binding site,
translation initiation signal, and, optionally, a repressor gene
or various activator genes.

       The recombinant expression vector carrying the DNA sequence
encoding a laccase variant of the invention may be any vector
20 which may conveniently be subjected to recombinant DNA
procedures, and the choice of vector will often depend on the
host cell into which it is to be introduced. Thus, the vector may
be an autonomously replicating vector, i.e. a vector which exists
as an extrachromosomal entity, the replication of which is
25 independent of chromosomal replication, e.g. a plasmid, a
bacteriophage or an extrachromosomal element, minichromosome or
an artificial chromosome. Alternatively, the vector may be one
which, when introduced into a host cell, is integrated into the
host cell genome and replicated together with the chromosome(s)
30 into which it has been integrated.

       In the vector, the DNA sequence should be operably connected
to a suitable promoter sequence. The promoter may be any DNA
sequence which shows transcriptional activity in the host cell of
choice and may be derived from genes encoding proteins either
35 homologous or heterologous to the host cell. Examples of suitable
promoters for directing the transcription of the DNA sequence
encoding a laccase variant of the invention, especially in a
fungal host, are those derived from the gene encoding *A. oryzae*

TAKA amylase, *Rhizomucor miehei* aspartic proteinase, A. *niger* neutral α-amylase, A. *niger* acid stable α-amylase, A. *niger* glucoamylase, *Rhizomucor miehei* lipase, A. *oryzae* alkaline protease, A. *oryzae* triose phosphate isomerase or A. *nidulans* acetamidase.

5   The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, polyadenylation sequences operably connected to the DNA sequence encoding the laccase variant of the invention. Termination and polyadenylation sequences may suitably be derived from the same sources as the promoter.

10 sources as the promoter.

The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

15   The vector may also comprise a selectable marker, e.g. a gene, the product of which complements a defect in the host cell, such as one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracyclin resistance. Furthermore, the vector may comprise *Aspergillus* selection markers

20 such as amdS, argB, niaD and sC, a marker giving rise to hygromycin resistance, or the selection may be accomplished by co-transformation, e.g. as described in WO 91/17243.

The procedures used to ligate the DNA construct of the invention encoding a laccase variant, the promoter, terminator and

25 other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

The cell of the invention, either comprising a DNA construct

30 or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of a laccase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or

35 more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of

the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in

5 connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a fungal cell.

The filamentous fungus may advantageously belong to a species

10 of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergillus niger*. Fungal cells may be transformed by a process involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells

15 is described in EP 238 023.

In a yet further aspect, the present invention relates to a method of producing a laccase variant of the invention, which method comprises cultivating a host cell as described above under conditions conducive to the production of the variant and

20 recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the laccase variant of the invention. Suitable media are available from commercial suppliers or may be

25 prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The laccase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by

30 centrifugation or filtration, and precipitating proteinaceous components of the medium by means of a salt such as ammonium sulphate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

35

Industrial Applications

The laccase variants of this invention possesses valuable properties allowing for various industrial applications, in

particular lignin modification, paper strengthening, dye transfer inhibition in detergents, phenol polymerization, hair dyeing, bleaching of textiles (in particular bleaching of denim as described in WO 96/12845 and WO 96/12846) and waste water
5 treatment. Any detergent composition normally used for enzymes may be used, e.g., the detergent compositions disclosed in WO 95/01426.

The invention is further illustrated in the following examples, which are not intended to be in any way limiting to the
10 scope of the invention as claimed.

EXAMPLE 1

Storage stability of the wild type *Myceliophthora thermophila*
15 and the *Polyporus pinsitus* laccases.

The storage stability of the *Myceliophthora thermophila* and the *Polyporus pinsitus* laccases was tested for 2 weeks at 40°C at pH 5, 8 and 9.3, respectively.

The laccase (1 mg/ml) was dialyzed against 0.1 M sodium
20 acetate, pH 5, or 0.1 M Tris-maleate, pH 8, or 0.1 M Tris-maleate, pH 9.3. Following dialysis the different preparations were poured into two sets of glass vials with screw caps: one for the liquid formulation and the other one for the lyophilized form. After two weeks of incubation the enzyme activity was
25 measured as described above and the residual activity of the enzymes was calculated in percentage using a preparation of *Myceliophthora thermophila* and *Polyporus pinsitus* kept at 4°C as references. The results are given below in Table 1 and 2.

30

Table 1 Storage stability of *Myceliophthora thermophila*

pH	Liquid formulation Residual activity (%)	Lyophilized form Residual activity (%)
5.0	<5	<5
8.0	<5	<5
9.3	35	30

Table 2 Storage stability of *Polyporus pinsitus*

pH	Liquid formulation Residual activity (%)	Lyophilized form Residual activity (%)
5.0	<5	n.d.
8.0	35	n.d.
9.3	n.d*	n.d.

* not determined

5 EXAMPLE 2

Homology building of the *Polyporus pinsitus* 3D-structure

        Using sequence homology of *Coprinus cinereus* (CcL) to other

sequences, e.g., *Polyporus pinsitus*, Coprinus-like 3 D-structures

10 can be found.

        In comparison with the *Coprinus cinereus*, used for

elucidating the structure, *Polyporus pinsitus* differs in a number

of residues. The model may be built using the HOMOLOGY program

from BIOSYM. The program substitutes the amino acids in the

15 *Coprinus cinereus* with amino acids from *Polyporus pinsitus* in the

homologous positions defined in the program as structurally

conserved regions (SCR). The residues in between are built using

the LOOP option with GENERATE. Using these steps a crude model

may be obtained which gives information of spatial interactions.

20   The structure can be refined using the method described in the

HOMOLOGY package.

EXAMPLE 3

25 Storage stability of *Myceliophthora thermophila* variants

    Laccase activity:

        In this Example the *Myceliophthora thermophila* laccase

variants were measured using 0.4 mM HEPO in 0.1 M Tris-maleate,

30 pH 7.5, 0.05% TWEEN-20 at 30°C. The absorbance at 528 nm was

followed for 200 s and the rate calculated from the linear part

of the progress curve.

The storage stability of the *Myceliophthora thermophila* variants were tested for 4 weeks at 40°C at pH 5, 7, and 9.3, respectively. The laccase (1 mg/ml) was dialyzed against 0.1 M
5 Tris-maleate, pH 5 or 0.1 M Tris-maleate, pH 7 or 0.1 M Tris-maleate, pH 9.3. Following dialysis the different preparations were poured into two set of glass vials with screw caps: one for the liquid formulation and the other set of glasses for lyophilization. Following two and four weeks of incubation the
10 enzyme activity was measured as described above and the residual activity of the variants were calculated in percentage using a preparation kept at 4°C as reference.

Table 3. Storage stability of *Myceliophthora thermophila*
15 variants, lyophilized formulation

	Residual activity, pH 5		Residual activity, pH 7		Residual activity, pH 9.2	
	2 weeks	4 weeks	2 weeks	4 weeks	2 weeks	4 weeks
wt	18	18	55	36	59	38
W136F	<5	<5	76	64	88	77
Y137F	12	<5	58	41	64	49
Y145F	<5	<5	53	20	45	51
W373F	14	14	33	19	51	36
M433I	7	<5	57	43	74	35
M480L	33	18	65	32	72	52
W507F	18	<5	72	51	68	71

In lyophilized form none of the tested variants have improved
20 stability at pH 5. At pH 7 and pH 9.2 both W136F and W507F have increased stability. At pH 9.2 M480L is also better than wt.

Table 4. Storage stability of *Myceliophthora thermophila* variants, liquid formulation

	Residual activity, pH 5, 2 weeks	pH	Residual activity, pH 7, 2 weeks	Residual activity, pH 9.2, 2 weeks
wt	<5		5	20
W136F	5		28	55
Y137F	<5		<5	<5
Y145F	<5		<5	<5
W373F	<5		40	<5
M433I	8		40	65
M480L	<5		<5	15
W507F	<5		<5	22

5   Also in the liquid formulation none of the tested variants have improved stability at pH 5. At pH 7 and pH 9.2 both W136F and M433I has increased stability. At pH7 W373F has better stability than wt but the variant looses the stability completely at pH 9.2.

10   Of the tested variants only W136F has increased stability in both formulations.

Appendix 1:

```
SEQRES   1 A  504  GLN ILE VAL ASN SER VAL ASP THR MET THR LEU THR ASN
SEQRES   2 A  504  ALA ASN VAL SER PRO ASP GLY PHE THR ARG ALA GLY ILE
SEQRES   3 A  504  LEU VAL ASN GLY VAL HIS GLY PRO LEU ILE ARG GLY GLY
SEQRES   4 A  504  LYS ASN ASP ASN PHE GLU LEU ASN VAL VAL ASN ASP LEU
SEQRES   5 A  504  ASP ASN PRO THR MET LEU ARG PRO THR SER ILE HIS TRP
SEQRES   6 A  504  HIS GLY LEU PHE GLN ARG GLY THR ASN TRP ALA ASN GLY
SEQRES   7 A  504  ALA ASP GLY VAL ASN GLN CYS PRO ILE SER PRO GLY HIS
SEQRES   8 A  504  ALA PHE LEU TYR LYS PHE THR PRO ALA GLY HIS ALA GLY
SEQRES   9 A  504  THR PHE TRP TYR HIS SER HIS PHE GLY THR GLN TYR CYS
SEQRES  10 A  504  ASP GLY LEU ARG GLY PRO MET VAL ILE TYR ASP ASP ASN
SEQRES  11 A  504  ASP PRO HIS ALA ALA LEU TYR ASP GLU ASP ASP GLU ASN
SEQRES  12 A  504  THR ILE ILE THR LEU ALA ASP TRP TYR HIS ILE PRO ALA
SEQRES  13 A  504  PRO SER ILE GLN GLY ALA ALA GLN PRO ASP ALA THR LEU
SEQRES  14 A  504  ILE ASN GLY LYS GLY ARG TYR VAL GLY GLY PRO ALA ALA
SEQRES  15 A  504  GLU LEU SER ILE VAL ASN VAL GLU GLN GLY LYS LYS TYR
SEQRES  16 A  504  ARG MET ARG LEU ILE SER LEU SER CYS ASP PRO ASN TRP
SEQRES  17 A  504  GLN PHE SER ILE ASP GLY HIS GLU LEU THR ILE ILE GLU
SEQRES  18 A  504  VAL ASP GLY ASN LEU THR GLU PRO HIS THR VAL ASP ARG
SEQRES  19 A  504  LEU GLN ILE PHE THR GLY GLN ARG TYR SER PHE VAL LEU
SEQRES  20 A  504  ASP ALA ASN GLN PRO VAL ASP ASN TYR TRP ILE ARG ALA
SEQRES  21 A  504  GLN PRO ASN LYS GLY ARG ASN GLY LEU ALA GLY THR PHE
SEQRES  22 A  504  ALA ASN GLY VAL ASN SER ALA ILE LEU ARG TYR ALA GLY
SEQRES  23 A  504  ALA ALA ASN ALA ASP PRO THR THR SER ALA ASN PRO ASN
SEQRES  24 A  504  PRO ALA GLN LEU ASN GLU ALA ASP LEU HIS ALA LEU ILE
SEQRES  25 A  504  ASP PRO ALA ALA PRO GLY ILE PRO THR PRO GLY ALA ALA
SEQRES  26 A  504  ASN VAL ASN LEU ARG PHE GLN LEU GLY PHE SER GLY GLY
SEQRES  27 A  504  ARG PHE THR ILE ASN GLY THR ALA TYR GLU SER PRO SER
SEQRES  28 A  504  VAL PRO THR LEU LEU GLN ILE MET SER GLY ALA GLN SER
SEQRES  29 A  504  ALA ASN ASP LEU LEU PRO ALA GLY SER VAL TYR GLU LEU
SEQRES  30 A  504  PRO ARG ASN GLN VAL VAL GLU LEU VAL VAL PRO ALA GLY
SEQRES  31 A  504  VAL LEU GLY GLY PRO HIS PRO PHE HIS LEU HIS GLY HIS
SEQRES  32 A  504  ALA PHE SER VAL VAL ARG SER ALA GLY SER SER THR TYR
SEQRES  33 A  504  ASN PHE VAL ASN PRO VAL LYS ARG ASP VAL VAL SER LEU
SEQRES  34 A  504  GLY VAL THR GLY ASP GLU VAL THR ILE ARG PHE VAL THR
SEQRES  35 A  504  ASP ASN PRO GLY PRO TRP PHE PHE HIS CYS HIS ILE GLU
SEQRES  36 A  504  PHE HIS LEU MET ASN GLY LEU ALA ILE VAL PHE ALA GLU
```

SEQRES 37 A 504 ASP MET ALA ASN THR VAL ASP ALA ASN ASN PRO PRO VAL

SEQRES 38 A 504 GLU TRP ALA GLN LEU CYS GLU ILE TYR ASP ASP LEU PRO

SEQRES 39 A 504 PRO GLU ALA THR SER ILE GLN THR VAL VAL

SSBOND 1 CYS   85 CYS   487

SSBOND 2 CYS   117 CYS   204

CRYST   45.390 85.720 143.070 90.00 90.00 90.00 P212121

SCALE1   0.02203 0.00000 0.00000   0.00000

SCALE2   0.00000 0.01167 0.00000   0.00000

SCALE3   0.00000 0.00000 0.00699   0.00000

ATOM   1 N   ALA A 1 0   18.748 34.495 5.326 1.00 36.36

ATOM   2 CA ALA A 1 0   19.554 35.757 5.185 1.00 35.87

ATOM   3 C   ALA A 1 0   19.785 36.380 6.558 1.00 34.53

ATOM   4 O   ALA A 1 0   19.248 35.884 7.577 1.00 35.40

ATOM   5 CB ALA A 1 0   19.050 36.675 4.107 1.00 36.65

ATOM   6 N   ILE A 2 0   20.844 37.201 6.659 1.00 31.00

ATOM   7 CA ILE A 2 0   21.310 37.654 7.963 1.00 27.71

ATOM   8 C   ILE A 2 0   21.368 39.165 8.117 1.00 25.19

ATOM   9 O   ILE A 2 0   21.789 39.861 7.192 1.00 23.77

ATOM   10 CB ILE A 2 0   22.744 37.107 8.206 1.00 28.28

ATOM   11 CG1 ILE A 2 0   22.790 35.590 8.022 1.00 28.54

ATOM   12 CG2 ILE A 2 0   23.285 37.557 9.554 1.00 27.91

ATOM   13 CD1 ILE A 2 0   23.334 34.738 9.130 1.00 29.32

ATOM   14 N   VAL A 3 0   20.986 39.659 9.283 1.00 22.31

ATOM   15 CA VAL A 3 0   21.093 41.092 9.540 1.00 22.78

ATOM   16 C   VAL A 3 0   22.246 41.297 10.524 1.00 22.62

ATOM   17 O   VAL A 3 0   22.460 40.556 11.467 1.00 21.74

ATOM   18 CB VAL A 3 0   19.801 41.849 9.799 1.00 23.54

ATOM   19 CG1 VAL A 3 0   18.537 40.985 9.684 1.00 21.30

ATOM   20 CG2 VAL A 3 0   19.760 42.709 11.055 1.00 21.32

ATOM   21 N   ASN A 4 0   23.122 42.261 10.209 1.00 23.39

ATOM   22 CA ASN A 4 0   24.303 42.520 11.021 1.00 23.45

ATOM   23 C   ASN A 4 0   24.002 43.517 12.126 1.00 24.44

ATOM   24 O   ASN A 4 0   22.928 44.122 12.160 1.00 23.05

ATOM   25 CB ASN A 4 0   25.477 42.965 10.149 1.00 24.77

ATOM   26 CG ASN A 4 0   25.726 41.991 9.021 1.00 26.62

ATOM   27 OD1 ASN A 4 0   25.668 42.388 7.849 1.00 30.29

ATOM   28 ND2 ASN A 4 0   25.923 40.719 9.324 1.00 27.59

ATOM   29 N   SER A 5 0   24.960 43.707 13.040 1.00 24.28

```
     ATOM   30 CA  SER A  5 0  24.702 44.636 14.143 1.00 25.77
     ATOM   31 C   SER A  5 0  24.595 46.090 13.701 1.00 24.41
     ATOM   32 O   SER A  5 0  23.973 46.862 14.452 1.00 23.55
     ATOM   33 CB  SER A  5 0  25.741 44.405 15.240 1.00 26.18
  5  ATOM   34 OG  SER A  5 0  26.976 44.750 14.641 1.00 27.89
     ATOM   35 N   VAL A  6 0  25.104 46.517 12.539 1.00 24.01
     ATOM   36 CA  VAL A  6 0  24.770 47.863 12.096 1.00 25.06
     ATOM   37 C   VAL A  6 0  24.131 47.617 10.731 1.00 25.57
     ATOM   38 O   VAL A  6 0  24.778 47.030  9.874 1.00 28.07
 10  ATOM   39 CB  VAL A  6 0  25.722 49.032 12.155 1.00 26.65
     ATOM   40 CG1 VAL A  6 0  26.937 48.759 13.025 1.00 26.73
     ATOM   41 CG2 VAL A  6 0  26.098 49.614 10.801 1.00 25.50
     ATOM   42 N   ASP A  7 0  22.848 47.952 10.605 1.00 23.82
     ATOM   43 CA  ASP A  7 0  22.173 47.543  9.369 1.00 24.07
 15  ATOM   44 C   ASP A  7 0  20.794 48.170  9.276 1.00 23.66
     ATOM   45 O   ASP A  7 0  20.342 48.845 10.204 1.00 23.47
     ATOM   46 CB  ASP A  7 0  21.996 46.012  9.444 1.00 23.43
     ATOM   47 CG  ASP A  7 0  22.017 45.317  8.111 1.00 23.78
     ATOM   48 OD1 ASP A  7 0  21.805 45.937  7.055 1.00 23.74
 20  ATOM   49 OD2 ASP A  7 0  22.255 44.089  8.099 1.00 24.62
     ATOM   50 N   THR A  8 0  20.155 47.881  8.158 1.00 23.88
     ATOM   51 CA  THR A  8 0  18.799 48.359  7.928 1.00 24.45
     ATOM   52 C   THR A  8 0  17.813 47.189  7.950 1.00 22.49
     ATOM   53 O   THR A  8 0  18.143 46.142  7.377 1.00 22.56
 25  ATOM   54 CB  THR A  8 0  18.694 49.108  6.579 1.00 25.75
     ATOM   55 OG1 THR A  8 0  19.573 50.242  6.719 1.00 28.53
     ATOM   56 CG2 THR A  8 0  17.295 49.656  6.339 1.00 25.55
     ATOM   57 N   MET A  9 0  16.677 47.364  8.602 1.00 19.10
     ATOM   58 CA  MET A  9 0  15.650 46.311  8.616 1.00 20.47
 30  ATOM   59 C   MET A  9 0  14.392 46.863  7.925 1.00 21.97
     ATOM   60 O   MET A  9 0  13.638 47.638  8.544 1.00 19.49
     ATOM   61 CB  MET A  9 0  15.308 45.871 10.022 1.00 20.49
     ATOM   62 CG  MET A  9 0  16.351 44.982 10.682 1.00 22.11
     ATOM   63 SD  MET A  9 0  16.192 44.917 12.482 1.00 24.71
 35  ATOM   64 CE  MET A  9 0  14.640 44.024 12.635 1.00 22.61
     ATOM   65 N   THR A 10 0  14.246 46.516  6.641 1.00 21.81
     ATOM   66 CA  THR A 10 0  13.073 47.064  5.926 1.00 23.43
     ATOM   67 C   THR A 10 0  11.912 46.081  6.046 1.00 22.90
```

```
    ATOM   68 O   THR A 10 0  12.056 44.890  5.719 1.00 23.55
    ATOM   69 CB  THR A 10 0  13.390 47.384  4.459 1.00 24.69
    ATOM   70 OG1 THR A 10 0  14.533 48.261  4.456 1.00 26.08
    ATOM   71 CG2 THR A 10 0  12.216 48.028  3.742 1.00 23.95
  5 ATOM   72 N   LEU A 11 0  10.820 46.600  6.583 1.00 21.13
    ATOM   73 CA  LEU A 11 0   9.615 45.836  6.846 1.00 21.10
    ATOM   74 C   LEU A 11 0   8.607 45.957  5.709 1.00 24.58
    ATOM   75 O   LEU A 11 0   8.124 47.056  5.358 1.00 23.89
    ATOM   76 CB  LEU A 11 0   9.045 46.411  8.129 1.00 21.29
 10 ATOM   77 CG  LEU A 11 0   9.474 45.955  9.508 1.00 22.26
    ATOM   78 CD1 LEU A 11 0  10.952 45.742  9.692 1.00 22.42
    ATOM   79 CD2 LEU A 11 0   8.978 46.931 10.583 1.00 22.75
    ATOM   80 N   THR A 12 0   8.272 44.836  5.057 1.00 24.01
    ATOM   81 CA  THR A 12 0   7.302 44.851  3.980 1.00 24.33
 15 ATOM   82 C   THR A 12 0   6.322 43.677  4.123 1.00 25.34
    ATOM   83 O   THR A 12 0   6.480 42.740  4.913 1.00 25.62
    ATOM   84 CB  THR A 12 0   7.882 44.776  2.560 1.00 25.12
    ATOM   85 OG1 THR A 12 0   8.575 43.548  2.377 1.00 24.05
    ATOM   86 CG2 THR A 12 0   8.847 45.905  2.217 1.00 25.26
 20 ATOM   87 N   ASN A 13 0   5.261 43.760  3.335 1.00 24.09
    ATOM   88 CA  ASN A 13 0   4.232 42.722  3.299 1.00 22.87
    ATOM   89 C   ASN A 13 0   4.422 41.954  1.989 1.00 22.13
    ATOM   90 O   ASN A 13 0   4.809 42.600  1.023 1.00 22.32
    ATOM   91 CB  ASN A 13 0   2.852 43.355  3.311 1.00 21.58
 25 ATOM   92 CG  ASN A 13 0   2.526 44.060  4.607 1.00 22.50
    ATOM   93 OD1 ASN A 13 0   2.187 45.245  4.648 1.00 22.20
    ATOM   94 ND2 ASN A 13 0   2.615 43.306  5.705 1.00 21.81
    ATOM   95 N   ALA A 14 0   4.218 40.655  1.985 1.00 21.00
    ATOM   96 CA  ALA A 14 0   4.270 39.869  0.762 1.00 21.93
 30 ATOM   97 C   ALA A 14 0   3.571 38.533  1.078 1.00 20.77
    ATOM   98 O   ALA A 14 0   3.292 38.309  2.259 1.00 20.45
    ATOM   99 CB  ALA A 14 0   5.676 39.618  0.248 1.00 23.72
    ATOM  100 N   ASN A 15 0   3.366 37.695  0.072 1.00 18.88
    ATOM  101 CA  ASN A 15 0   2.748 36.412  0.337 1.00 19.67
 35 ATOM  102 C   ASN A 15 0   3.798 35.457  0.873 1.00 19.19
    ATOM  103 O   ASN A 15 0   4.891 35.474  0.338 1.00 19.57
    ATOM  104 CB  ASN A 15 0   2.114 35.721 -0.875 1.00 21.13
    ATOM  105 CG  ASN A 15 0   0.839 36.457 -1.284 1.00 21.15
```

```
      ATOM   106 OD1 ASN A 15 0   0.343 37.207 -0.472 1.00 20.87
      ATOM   107 ND2 ASN A 15 0   0.379 36.284 -2.501 1.00 20.00
      ATOM   108 N   VAL A 16 0   3.358 34.614  1.772 1.00 19.11
      ATOM   109 CA  VAL A 16 0   4.322 33.628  2.342 1.00 18.90
  5   ATOM   110 C   VAL A 16 0   3.626 32.293  2.345 1.00 19.25
      ATOM   111 O   VAL A 16 0   2.386 32.281  2.406 1.00 16.71
      ATOM   112 CB  VAL A 16 0   4.612 34.317  3.691 1.00 19.95
      ATOM   113 CG1 VAL A 16 0   3.990 33.749  4.937 1.00 18.58
      ATOM   114 CG2 VAL A 16 0   6.091 34.603  3.814 1.00 21.38
 10   ATOM   115 N   SER A 17 0   4.312 31.157  2.303 1.00 18.57
      ATOM   116 CA  SER A 17 0   3.678 29.869  2.410 1.00 20.90
      ATOM   117 C   SER A 17 0   4.608 28.866  3.065 1.00 21.12
      ATOM   118 O   SER A 17 0   5.106 27.939  2.448 1.00 21.24
      ATOM   119 CB  SER A 17 0   3.186 29.285  1.080 1.00 23.95
 15   ATOM   120 OG  SER A 17 0   4.204 29.399  0.125 1.00 26.79
      ATOM   121 N   PRO A 18 0   4.834 29.051  4.358 1.00 20.78
      ATOM   122 CA  PRO A 18 0   5.703 28.216  5.141 1.00 20.02
      ATOM   123 C   PRO A 18 0   5.197 26.793  5.376 1.00 19.74
      ATOM   124 O   PRO A 18 0   5.978 25.920  5.753 1.00 17.97
 20   ATOM   125 CB  PRO A 18 0   5.889 28.954  6.481 1.00 19.27
      ATOM   126 CG  PRO A 18 0   4.701 29.832  6.536 1.00 21.41
      ATOM   127 CD  PRO A 18 0   4.249 30.153  5.128 1.00 20.70
      ATOM   128 N   ASP A 19 0   3.899 26.534  5.241 1.00 18.82
      ATOM   129 CA  ASP A 19 0   3.323 25.227  5.475 1.00 16.87
 25   ATOM   130 C   ASP A 19 0   2.548 24.823  4.237 1.00 17.28
      ATOM   131 O   ASP A 19 0   1.713 23.929  4.337 1.00 17.84
      ATOM   132 CB  ASP A 19 0   2.419 25.207  6.701 1.00 16.54
      ATOM   133 CG  ASP A 19 0   1.192 26.120  6.596 1.00 16.67
      ATOM   134 OD1 ASP A 19 0   1.032 26.935  5.654 1.00 14.17
 30   ATOM   135 OD2 ASP A 19 0   0.360 26.045  7.529 1.00 14.56
      ATOM   136 N   GLY A 20 0   2.782 25.469  3.100 1.00 17.87
      ATOM   137 CA  GLY A 20 0   2.079 25.091  1.890 1.00 19.40
      ATOM   138 C   GLY A 20 0   0.732 25.789  1.699 1.00 22.52
      ATOM   139 O   GLY A 20 0   0.158 25.619  0.628 1.00 22.87
 35   ATOM   140 N   PHE A 21 0   0.240 26.587  2.631 1.00 21.35
      ATOM   141 CA  PHE A 21 0  -0.913 27.443  2.534 1.00 20.39
      ATOM   142 C   PHE A 21 0  -0.348 28.855  2.322 1.00 21.23
      ATOM   143 O   PHE A 21 0   0.475 29.316  3.122 1.00 21.26
```

```
    ATOM  144 CB  PHE A 21 0  -1.742 27.472  3.814 1.00 20.80
    ATOM  145 CG  PHE A 21 0  -3.059 28.180  3.695 1.00 21.91
    ATOM  146 CD1 PHE A 21 0  -3.171 29.527  3.963 1.00 22.49
    ATOM  147 CD2 PHE A 21 0  -4.207 27.470  3.327 1.00 22.51
 5  ATOM  148 CE1 PHE A 21 0  -4.370 30.207  3.845 1.00 22.27
    ATOM  149 CE2 PHE A 21 0  -5.419 28.128  3.203 1.00 22.79
    ATOM  150 CZ  PHE A 21 0  -5.498 29.497  3.474 1.00 23.34
    ATOM  151 N   THR A 22 0  -0.638 29.514  1.225 1.00 20.20
    ATOM  152 CA  THR A 22 0  -0.143 30.850  0.977 1.00 21.36
10  ATOM  153 C   THR A 22 0  -1.083 31.939  1.488 1.00 21.79
    ATOM  154 O   THR A 22 0  -2.271 31.952  1.162 1.00 21.19
    ATOM  155 CB  THR A 22 0   0.045 31.012 -0.553 1.00 21.46
    ATOM  156 OG1 THR A 22 0   0.838 29.881 -0.934 1.00 20.09
    ATOM  157 CG2 THR A 22 0   0.693 32.353 -0.891 1.00 20.94
15  ATOM  158 N   ARG A 23 0  -0.562 32.871  2.257 1.00 20.80
    ATOM  159 CA  ARG A 23 0  -1.230 34.008  2.844 1.00 20.78
    ATOM  160 C   ARG A 23 0  -0.257 35.189  2.960 1.00 21.15
    ATOM  161 O   ARG A 23 0   0.954 35.018  2.740 1.00 20.42
    ATOM  162 CB  ARG A 23 0  -1.874 33.685  4.172 1.00 20.47
20  ATOM  163 CG  ARG A 23 0  -0.964 33.152  5.295 1.00 21.52
    ATOM  164 CD  ARG A 23 0  -0.552 34.357  6.113 1.00 22.75
    ATOM  165 NE  ARG A 23 0  -0.905 34.419  7.477 1.00 21.60
    ATOM  166 CZ  ARG A 23 0  -0.870 35.283  8.464 1.00 19.89
    ATOM  167 NH1 ARG A 23 0  -0.526 36.565  8.453 1.00 20.19
25  ATOM  168 NH2 ARG A 23 0  -1.249 34.744  9.610 1.00 18.64
    ATOM  169 N   ALA A 24 0  -0.784 36.389  3.199 1.00 20.05
    ATOM  170 CA  ALA A 24 0   0.140 37.541  3.243 1.00 22.03
    ATOM  171 C   ALA A 24 0   0.786 37.561  4.635 1.00 21.09
    ATOM  172 O   ALA A 24 0   0.200 37.124  5.637 1.00 21.16
30  ATOM  173 CB  ALA A 24 0  -0.578 38.836  2.902 1.00 22.98
    ATOM  174 N   GLY A 25 0   2.042 37.984  4.683 1.00 20.28
    ATOM  175 CA  GLY A 25 0   2.786 37.993  5.950 1.00 20.29
    ATOM  176 C   GLY A 25 0   3.649 39.254  5.979 1.00 21.38
    ATOM  177 O   GLY A 25 0   3.465 40.229  5.238 1.00 21.06
35  ATOM  178 N   ILE A 26 0   4.604 39.221  6.897 1.00 20.33
    ATOM  179 CA  ILE A 26 0   5.475 40.365  7.145 1.00 20.64
    ATOM  180 C   ILE A 26 0   6.903 39.886  6.932 1.00 20.00
    ATOM  181 O   ILE A 26 0   7.247 38.851  7.485 1.00 21.34
```

```
   ATOM  182 CB  ILE A 26  0   5.278 40.933  8.564 1.00 20.38
   ATOM  183 CG1 ILE A 26  0   3.883 41.536  8.667 1.00 20.72
   ATOM  184 CG2 ILE A 26  0   6.333 42.007  8.821 1.00 22.34
   ATOM  185 CD1 ILE A 26  0   3.310 41.822 10.024 1.00 20.76
 5 ATOM  186 N   LEU A 27  0   7.644 40.551  6.079 1.00 19.10
   ATOM  187 CA  LEU A 27  0   9.005 40.168  5.739 1.00 19.67
   ATOM  188 C   LEU A 27  0   9.964 41.226  6.280 1.00 19.85
   ATOM  189 O   LEU A 27  0   9.591 42.407  6.356 1.00 19.19
   ATOM  190 CB  LEU A 27  0   9.138 40.172  4.219 1.00 20.26
10 ATOM  191 CG  LEU A 27  0   9.046 38.883  3.415 1.00 22.65
   ATOM  192 CD1 LEU A 27  0   8.127 37.835  3.989 1.00 21.10
   ATOM  193 CD2 LEU A 27  0   8.738 39.198  1.963 1.00 22.01
   ATOM  194 N   VAL A 28  0  11.162 40.804  6.630 1.00 18.03
   ATOM  195 CA  VAL A 28  0  12.199 41.723  7.088 1.00 17.24
15 ATOM  196 C   VAL A 28  0  13.289 41.573  6.040 1.00 18.99
   ATOM  197 O   VAL A 28  0  13.791 40.453  5.863 1.00 20.36
   ATOM  198 CB  VAL A 28  0  12.762 41.415  8.491 1.00 16.50
   ATOM  199 CG1 VAL A 28  0  13.899 42.361  8.845 1.00 15.41
   ATOM  200 CG2 VAL A 28  0  11.681 41.517  9.558 1.00 15.42
20 ATOM  201 N   ASN A 29  0  13.575 42.601  5.256 1.00 20.78
   ATOM  202 CA  ASN A 29  0  14.567 42.579  4.198 1.00 20.46
   ATOM  203 C   ASN A 29  0  14.316 41.435  3.226 1.00 23.05
   ATOM  204 O   ASN A 29  0  15.247 40.675  2.880 1.00 23.62
   ATOM  205 CB  ASN A 29  0  15.982 42.446  4.764 1.00 21.06
25 ATOM  206 CG  ASN A 29  0  16.475 43.654  5.522 1.00 22.44
   ATOM  207 OD1 ASN A 29  0  15.870 44.722  5.434 1.00 23.47
   ATOM  208 ND2 ASN A 29  0  17.560 43.507  6.288 1.00 22.23
   ATOM  209 N   GLY A 30  0  13.053 41.215  2.878 1.00 23.18
   ATOM  210 CA  GLY A 30  0  12.662 40.181  1.922 1.00 23.36
30 ATOM  211 C   GLY A 30  0  12.723 38.757  2.436 1.00 23.85
   ATOM  212 O   GLY A 30  0  12.707 37.814  1.633 1.00 25.17
   ATOM  213 N   VAL A 31  0  12.832 38.585  3.755 1.00 21.85
   ATOM  214 CA  VAL A 31  0  12.999 37.276  4.352 1.00 20.55
   ATOM  215 C   VAL A 31  0  12.031 37.190  5.548 1.00 19.91
35 ATOM  216 O   VAL A 31  0  11.796 38.172  6.269 1.00 17.50
   ATOM  217 CB  VAL A 31  0  14.436 37.020  4.856 1.00 21.36
   ATOM  218 CG1 VAL A 31  0  14.556 35.709  5.626 1.00 20.79
   ATOM  219 CG2 VAL A 31  0  15.495 37.005  3.757 1.00 21.84
```

```
   ATOM   220 N   HIS A 32 0  11.489 35.984  5.698 1.00 17.05
   ATOM   221 CA  HIS A 32 0  10.592 35.729  6.797 1.00 18.61
   ATOM   222 C   HIS A 32 0  11.417 35.499  8.050 1.00 17.67
   ATOM   223 O   HIS A 32 0  11.873 34.385  8.216 1.00 18.72
 5 ATOM   224 CB  HIS A 32 0   9.676 34.543  6.493 1.00 21.00
   ATOM   225 CG  HIS A 32 0   8.639 34.208  7.517 1.00 23.80
   ATOM   226 ND1 HIS A 32 0   7.744 33.174  7.332 1.00 25.14
   ATOM   227 CD2 HIS A 32 0   8.331 34.720  8.735 1.00 25.32
   ATOM   228 CE1 HIS A 32 0   6.942 33.061  8.385 1.00 25.36
10 ATOM   229 NE2 HIS A 32 0   7.271 33.986  9.260 1.00 26.23
   ATOM   230 N   GLY A 33 0  11.522 36.446  8.960 1.00 16.23
   ATOM   231 CA  GLY A 33 0  12.276 36.252 10.198 1.00 16.97
   ATOM   232 C   GLY A 33 0  13.740 35.869 10.083 1.00 15.54
   ATOM   233 O   GLY A 33 0  14.228 34.885 10.609 1.00 15.13
15 ATOM   234 N   PRO A 34 0  14.555 36.734  9.475 1.00 15.75
   ATOM   235 CA  PRO A 34 0  16.012 36.561  9.359 1.00 14.70
   ATOM   236 C   PRO A 34 0  16.734 36.660 10.701 1.00 14.02
   ATOM   237 O   PRO A 34 0  16.241 37.252 11.673 1.00 10.44
   ATOM   238 CB  PRO A 34 0  16.491 37.699  8.435 1.00 14.40
20 ATOM   239 CG  PRO A 34 0  15.441 38.742  8.783 1.00 15.11
   ATOM   240 CD  PRO A 34 0  14.113 38.005  8.905 1.00 13.69
   ATOM   241 N   LEU A 35 0  17.925 36.049 10.767 1.00 13.60
   ATOM   242 CA  LEU A 35 0  18.748 36.022 11.963 1.00 14.35
   ATOM   243 C   LEU A 35 0  19.462 37.359 12.161 1.00 16.25
25 ATOM   244 O   LEU A 35 0  20.015 37.902 11.210 1.00 14.10
   ATOM   245 CB  LEU A 35 0  19.834 34.916 11.862 1.00 15.33
   ATOM   246 CG  LEU A 35 0  20.958 34.943 12.911 1.00 17.74
   ATOM   247 CD1 LEU A 35 0  20.486 34.698 14.348 1.00 16.30
   ATOM   248 CD2 LEU A 35 0  22.052 33.934 12.575 1.00 16.60
30 ATOM   249 N   ILE A 36 0  19.471 37.855 13.384 1.00 16.71
   ATOM   250 CA  ILE A 36 0  20.265 39.027 13.738 1.00 16.66
   ATOM   251 C   ILE A 36 0  21.403 38.487 14.620 1.00 17.92
   ATOM   252 O   ILE A 36 0  21.183 37.732 15.573 1.00 17.20
   ATOM   253 CB  ILE A 36 0  19.560 40.129 14.533 1.00 16.60
35 ATOM   254 CG1 ILE A 36 0  18.389 40.771 13.771 1.00 16.09
   ATOM   255 CG2 ILE A 36 0  20.565 41.226 14.917 1.00 17.67
   ATOM   256 CD1 ILE A 36 0  17.590 41.754 14.629 1.00 15.88
   ATOM   257 N   ARG A 37 0  22.647 38.829 14.288 1.00 18.72
```

```
   ATOM   258 CA  ARG A 37  0  23.754 38.315 15.091 1.00 19.94
   ATOM   259 C   ARG A 37  0  24.839 39.369 15.280 1.00 20.08
   ATOM   260 O   ARG A 37  0  24.979 40.249 14.450 1.00 20.52
   ATOM   261 CB  ARG A 37  0  24.395 37.077 14.465 1.00 21.72
 5 ATOM   262 CG  ARG A 37  0  25.102 37.393 13.171 1.00 24.46
   ATOM   263 CD  ARG A 37  0  26.113 36.339 12.762 1.00 26.90
   ATOM   264 NE  ARG A 37  0  26.584 36.571 11.381 1.00 29.30
   ATOM   265 CZ  ARG A 37  0  26.838 35.571 10.528 1.00 31.29
   ATOM   266 NH1 ARG A 37  0  26.711 34.283 10.851 1.00 31.37
10 ATOM   267 NH2 ARG A 37  0  27.252 35.827  9.291 1.00 31.66
   ATOM   268 N   GLY A 38  0  25.587 39.223 16.361 1.00 20.22
   ATOM   269 CA  GLY A 38  0  26.716 40.121 16.611 1.00 18.98
   ATOM   270 C   GLY A 38  0  27.533 39.545 17.765 1.00 18.08
   ATOM   271 O   GLY A 38  0  27.259 38.421 18.225 1.00 15.92
15 ATOM   272 N   GLY A 39  0  28.436 40.412 18.238 1.00 17.65
   ATOM   273 CA  GLY A 39  0  29.322 40.026 19.351 1.00 16.23
   ATOM   274 C   GLY A 39  0  28.861 40.774 20.592 1.00 17.21
   ATOM   275 O   GLY A 39  0  28.157 41.784 20.489 1.00 17.27
   ATOM   276 N   LYS A 40  0  29.276 40.328 21.764 1.00 16.58
20 ATOM   277 CA  LYS A 40  0  28.839 40.805 23.057 1.00 18.03
   ATOM   278 C   LYS A 40  0  29.185 42.267 23.348 1.00 20.44
   ATOM   279 O   LYS A 40  0  28.562 42.878 24.221 1.00 19.42
   ATOM   280 CB  LYS A 40  0  29.394 39.933 24.185 1.00 16.74
   ATOM   281 CG  LYS A 40  0  30.892 39.997 24.370 1.00 17.98
25 ATOM   282 CD  LYS A 40  0  31.333 39.170 25.569 1.00 20.66
   ATOM   283 CE  LYS A 40  0  32.809 38.768 25.493 1.00 21.70
   ATOM   284 NZ  LYS A 40  0  33.227 38.111 26.757 1.00 23.11
   ATOM   285 N   ASN A 41  0  30.181 42.780 22.645 1.00 21.43
   ATOM   286 CA  ASN A 41  0  30.536 44.171 22.840 1.00 25.14
30 ATOM   287 C   ASN A 41  0  30.092 44.976 21.644 1.00 24.05
   ATOM   288 O   ASN A 41  0  30.409 46.161 21.655 1.00 25.66
   ATOM   289 CB  ASN A 41  0  32.052 44.326 23.111 1.00 27.02
   ATOM   290 CG  ASN A 41  0  32.434 43.606 24.404 1.00 29.76
   ATOM   291 OD1 ASN A 41  0  33.398 42.832 24.431 1.00 31.54
35 ATOM   292 ND2 ASN A 41  0  31.663 43.825 25.473 1.00 30.13
   ATOM   293 N   ASP A 42  0  29.424 44.447 20.631 1.00 23.80
   ATOM   294 CA  ASP A 42  0  29.073 45.325 19.506 1.00 24.12
   ATOM   295 C   ASP A 42  0  28.169 46.484 19.891 1.00 24.24
```

ATOM   296 O   ASP A 42 0 27.420 46.428 20.872 1.00 22.42
ATOM   297 CB ASP A 42 0 28.388 44.528 18.392 1.00 26.65
ATOM   298 CG ASP A 42 0 29.404 43.599 17.773 1.00 28.94
ATOM   299 OD1 ASP A 42 0 30.603 43.754 18.056 1.00 31.45
5 ATOM   300 OD2 ASP A 42 0 29.026 42.708 17.009 1.00 31.69
ATOM   301 N   ASN A 43 0 28.258 47.547 19.090 1.00 24.72
ATOM   302 CA ASN A 43 0 27.316 48.660 19.255 1.00 26.50
ATOM   303 C   ASN A 43 0 26.293 48.430 18.128 1.00 26.23
ATOM   304 O   ASN A 43 0 26.723 48.420 16.979 1.00 25.02
10 ATOM 305 CB ASN A 43 0 27.934 50.047 19.128 1.00 28.45
ATOM   306 CG ASN A 43 0 28.858 50.244 20.323 1.00 31.09
ATOM   307 OD1 ASN A 43 0 30.041 50.502 20.106 1.00 33.11
ATOM   308 ND2 ASN A 43 0 28.364 50.055 21.531 1.00 31.18
ATOM   309 N   PHE A 44 0 25.039 48.155 18.468 1.00 24.63
15 ATOM 310 CA PHE A 44 0 24.083 47.897 17.393 1.00 23.28
ATOM   311 C   PHE A 44 0 23.450 49.191 16.916 1.00 22.36
ATOM   312 O   PHE A 44 0 23.024 50.008 17.735 1.00 21.07
ATOM   313 CB PHE A 44 0 22.959 46.965 17.853 1.00 22.04
ATOM   314 CG PHE A 44 0 23.376 45.525 17.955 1.00 22.96
20 ATOM 315 CD1 PHE A 44 0 22.779 44.562 17.153 1.00 23.91
ATOM   316 CD2 PHE A 44 0 24.330 45.120 18.869 1.00 22.03
ATOM   317 CE1 PHE A 44 0 23.131 43.230 17.253 1.00 24.42
ATOM   318 CE2 PHE A 44 0 24.689 43.797 18.974 1.00 23.25
ATOM   319 CZ PHE A 44 0 24.095 42.837 18.168 1.00 24.02
25 ATOM 320 N   GLU A 45 0 23.350 49.343 15.604 1.00 22.78
ATOM   321 CA GLU A 45 0 22.611 50.482 15.054 1.00 24.47
ATOM   322 C   GLU A 45 0 21.619 49.884 14.055 1.00 23.79
ATOM   323 O   GLU A 45 0 22.017 49.587 12.924 1.00 24.40
ATOM   324 CB GLU A 45 0 23.543 51.473 14.368 1.00 27.07
30 ATOM 325 CG GLU A 45 0 24.474 52.130 15.374 1.00 31.60
ATOM   326 CD GLU A 45 0 25.380 53.179 14.772 1.00 33.90
ATOM   327 OE1 GLU A 45 0 25.354 53.438 13.559 1.00 35.62
ATOM   328 OE2 GLU A 45 0 26.155 53.748 15.565 1.00 36.42
ATOM   329 N   LEU A 46 0 20.369 49.684 14.465 1.00 22.18
35 ATOM 330 CA LEU A 46 0 19.419 49.044 13.556 1.00 21.22
ATOM   331 C   LEU A 46 0 18.348 50.001 13.077 1.00 21.27
ATOM   332 O   LEU A 46 0 17.464 50.429 13.812 1.00 21.60
ATOM   333 CB LEU A 46 0 18.837 47.811 14.262 1.00 20.72

```
   ATOM   334 CG  LEU A  46  0   19.827 46.658 14.403 1.00 21.28
   ATOM   335 CD1 LEU A  46  0   19.334 45.621 15.397 1.00 20.83
   ATOM   336 CD2 LEU A  46  0   20.148 46.034 13.052 1.00 18.33
   ATOM   337 N   ASN A  47  0   18.438 50.403 11.823 1.00 21.09
 5 ATOM   338 CA  ASN A  47  0   17.498 51.344 11.252 1.00 22.37
   ATOM   339 C   ASN A  47  0   16.273 50.558 10.803 1.00 22.18
   ATOM   340 O   ASN A  47  0   16.390 49.810  9.847 1.00 23.41
   ATOM   341 CB  ASN A  47  0   18.131 52.104 10.066 1.00 24.01
   ATOM   342 CG  ASN A  47  0   17.226 53.243  9.615 1.00 25.54
10 ATOM   343 OD1 ASN A  47  0   16.443 53.772 10.413 1.00 26.53
   ATOM   344 ND2 ASN A  47  0   17.332 53.612  8.346 1.00 26.01
   ATOM   345 N   VAL A  48  0   15.147 50.692 11.475 1.00 22.04
   ATOM   346 CA  VAL A  48  0   13.918 49.995 11.140 1.00 21.99
   ATOM   347 C   VAL A  48  0   13.026 50.879 10.269 1.00 21.82
15 ATOM   348 O   VAL A  48  0   12.532 51.910 10.699 1.00 20.61
   ATOM   349 CB  VAL A  48  0   13.176 49.579 12.430 1.00 22.64
   ATOM   350 CG1 VAL A  48  0   11.819 48.931 12.148 1.00 21.99
   ATOM   351 CG2 VAL A  48  0   14.098 48.631 13.216 1.00 21.68
   ATOM   352 N   VAL A  49  0   12.931 50.512  9.009 1.00 21.79
20 ATOM   353 CA  VAL A  49  0   12.164 51.167  7.966 1.00 21.34
   ATOM   354 C   VAL A  49  0   10.816 50.460  7.795 1.00 21.12
   ATOM   355 O   VAL A  49  0   10.703 49.308  7.365 1.00 19.76
   ATOM   356 CB  VAL A  49  0   12.983 51.189  6.665 1.00 22.02
   ATOM   357 CG1 VAL A  49  0   12.267 51.913  5.519 1.00 21.70
25 ATOM   358 CG2 VAL A  49  0   14.312 51.933  6.906 1.00 21.47
   ATOM   359 N   ASN A  50  0    9.767 51.112  8.257 1.00 20.26
   ATOM   360 CA  ASN A  50  0    8.424 50.611  8.215 1.00 22.70
   ATOM   361 C   ASN A  50  0    7.751 50.899  6.869 1.00 25.99
   ATOM   362 O   ASN A  50  0    7.043 51.925  6.735 1.00 27.06
30 ATOM   363 CB  ASN A  50  0    7.549 51.230  9.318 1.00 21.92
   ATOM   364 CG  ASN A  50  0    6.198 50.569  9.471 1.00 22.44
   ATOM   365 OD1 ASN A  50  0    5.818 49.801  8.572 1.00 24.19
   ATOM   366 ND2 ASN A  50  0    5.435 50.833 10.526 1.00 20.19
   ATOM   367 N   ASP A  51  0    7.915 49.959  5.926 1.00 26.42
35 ATOM   368 CA  ASP A  51  0    7.208 50.071  4.641 1.00 26.35
   ATOM   369 C   ASP A  51  0    5.951 49.200  4.600 1.00 24.86
   ATOM   370 O   ASP A  51  0    5.542 48.810  3.511 1.00 25.19
   ATOM   371 CB  ASP A  51  0    8.126 49.698  3.481 1.00 26.75
```

```
   ATOM    372 CG  ASP A 51 0    9.152 50.761  3.158 1.00 29.77
   ATOM    373 OD1 ASP A 51 0    8.944 51.904  3.617 1.00 31.03
   ATOM    374 OD2 ASP A 51 0   10.166 50.509  2.465 1.00 30.42
   ATOM    375 N   LEU A 52 0    5.332 48.801  5.700 1.00 25.05
 5 ATOM    376 CA  LEU A 52 0    4.172 47.911  5.640 1.00 25.44
   ATOM    377 C   LEU A 52 0    2.934 48.624  5.094 1.00 26.65
   ATOM    378 O   LEU A 52 0    2.553 49.696  5.586 1.00 24.56
   ATOM    379 CB  LEU A 52 0    3.837 47.374  7.029 1.00 24.19
   ATOM    380 CG  LEU A 52 0    4.896 46.503  7.699 1.00 24.60
10 ATOM    381 CD1 LEU A 52 0    4.611 46.424  9.196 1.00 24.05
   ATOM    382 CD2 LEU A 52 0    4.891 45.119  7.061 1.00 23.49
   ATOM    383 N   ASP A 53 0    2.242 47.980  4.169 1.00 28.79
   ATOM    384 CA  ASP A 53 0    1.049 48.602  3.581 1.00 29.91
   ATOM    385 C   ASP A 53 0   -0.135 47.658  3.492 1.00 29.90
15 ATOM    386 O   ASP A 53 0   -1.152 48.082  2.951 1.00 30.40
   ATOM    387 CB  ASP A 53 0    1.367 49.190  2.197 1.00 29.26
   ATOM    388 CG  ASP A 53 0    1.838 48.140  1.218 1.00 31.28
   ATOM    389 OD1 ASP A 53 0    1.865 46.926  1.540 1.00 31.64
   ATOM    390 OD2 ASP A 53 0    2.233 48.474  0.074 1.00 32.42
20 ATOM    391 N   ASN A 54 0   -0.060 46.437  4.014 1.00 29.44
   ATOM    392 CA  ASN A 54 0   -1.237 45.554  3.983 1.00 26.89
   ATOM    393 C   ASN A 54 0   -2.089 45.832  5.192 1.00 27.37
   ATOM    394 O   ASN A 54 0   -1.772 45.528  6.350 1.00 27.99
   ATOM    395 CB  ASN A 54 0   -0.831 44.095  3.913 1.00 25.11
25 ATOM    396 CG  ASN A 54 0   -1.978 43.141  3.690 1.00 24.20
   ATOM    397 OD1 ASN A 54 0   -1.874 42.344  2.746 1.00 25.13
   ATOM    398 ND2 ASN A 54 0   -3.030 43.182  4.481 1.00 23.26
   ATOM    399 N   PRO A 55 0   -3.337 46.256  4.961 1.00 28.44
   ATOM    400 CA  PRO A 55 0   -4.286 46.589  6.014 1.00 26.57
30 ATOM    401 C   PRO A 55 0   -4.909 45.414  6.723 1.00 27.10
   ATOM    402 O   PRO A 55 0   -5.671 45.624  7.687 1.00 26.05
   ATOM    403 CB  PRO A 55 0   -5.368 47.465  5.334 1.00 28.18
   ATOM    404 CG  PRO A 55 0   -5.249 47.049  3.899 1.00 27.50
   ATOM    405 CD  PRO A 55 0   -3.844 46.564  3.625 1.00 27.56
35 ATOM    406 N   THR A 56 0   -4.603 44.160  6.345 1.00 25.55
   ATOM    407 CA  THR A 56 0   -5.214 43.024  7.065 1.00 25.52
   ATOM    408 C   THR A 56 0   -4.446 42.647  8.326 1.00 24.87
   ATOM    409 O   THR A 56 0   -4.766 41.764  9.115 1.00 23.97
```

```
    ATOM   410 CB  THR A 56  0   -5.393  41.807   6.154  1.00 25.10
    ATOM   411 OG1 THR A 56  0   -4.100  41.345   5.763  1.00 24.26
    ATOM   412 CG2 THR A 56  0   -6.178  42.123   4.861  1.00 25.63
    ATOM   413 N   MET A 57  0   -3.317  43.311   8.558  1.00 26.01
  5 ATOM   414 CA  MET A 57  0   -2.553  43.099   9.801  1.00 26.57
    ATOM   415 C   MET A 57  0   -2.026  44.475  10.201  1.00 25.88
    ATOM   416 O   MET A 57  0   -2.026  45.416   9.397  1.00 25.18
    ATOM   417 CB  MET A 57  0   -1.561  41.939   9.698  1.00 25.42
    ATOM   418 CG  MET A 57  0   -0.639  41.868   8.554  1.00 24.37
 10 ATOM   419 SD  MET A 57  0   -0.034  40.288   7.916  1.00 22.34
    ATOM   420 CE  MET A 57  0   -0.275  40.640   6.167  1.00 19.23
    ATOM   421 N   LEU A 58  0   -1.694  44.601  11.476  1.00 25.98
    ATOM   422 CA  LEU A 58  0   -1.180  45.850  12.036  1.00 25.57
    ATOM   423 C   LEU A 58  0   -0.053  46.425  11.195  1.00 24.52
 15 ATOM   424 O   LEU A 58  0    0.824  45.739  10.638  1.00 23.63
    ATOM   425 CB  LEU A 58  0   -0.757  45.535  13.463  1.00 26.67
    ATOM   426 CG  LEU A 58  0   -1.628  45.817  14.657  1.00 28.97
    ATOM   427 CD1 LEU A 58  0   -3.107  45.995  14.312  1.00 30.99
    ATOM   428 CD2 LEU A 58  0   -1.488  44.756  15.736  1.00 28.36
 20 ATOM   429 N   ARG A 59  0   -0.078  47.741  11.030  1.00 24.96
    ATOM   430 CA  ARG A 59  0    0.918  48.434  10.231  1.00 26.92
    ATOM   431 C   ARG A 59  0    1.932  49.229  11.014  1.00 26.31
    ATOM   432 O   ARG A 59  0    3.120  49.198  10.699  1.00 28.82
    ATOM   433 CB  ARG A 59  0    0.260  49.277   9.132  1.00 28.35
 25 ATOM   434 CG  ARG A 59  0   -0.252  48.385   7.986  1.00 29.50
    ATOM   435 CD  ARG A 59  0   -0.986  49.274   6.996  1.00 30.33
    ATOM   436 NE  ARG A 59  0   -2.333  49.604   7.459  1.00 32.26
    ATOM   437 CZ  ARG A 59  0   -3.121  50.525   6.883  1.00 33.24
    ATOM   438 NH1 ARG A 59  0   -2.679  51.233   5.845  1.00 32.27
 30 ATOM   439 NH2 ARG A 59  0   -4.340  50.712   7.389  1.00 32.65
    ATOM   440 N   PRO A 60  0    1.542  49.961  12.020  1.00 26.30
    ATOM   441 CA  PRO A 60  0    2.460  50.669  12.916  1.00 26.19
    ATOM   442 C   PRO A 60  0    3.312  49.591  13.595  1.00 25.29
    ATOM   443 O   PRO A 60  0    2.879  48.432  13.668  1.00 24.63
 35 ATOM   444 CB  PRO A 60  0    1.623  51.464  13.925  1.00 25.93
    ATOM   445 CG  PRO A 60  0    0.235  51.357  13.325  1.00 26.19
    ATOM   446 CD  PRO A 60  0    0.165  50.073  12.508  1.00 26.23
    ATOM   447 N   THR A 61  0    4.544  49.932  13.976  1.00 24.60
```

```
     ATOM   448 CA  THR A  61  0   5.365 48.871 14.587 1.00 23.49
     ATOM   449 C   THR A  61  0   6.204 49.400 15.743 1.00 22.83
     ATOM   450 O   THR A  61  0   6.390 50.601 15.921 1.00 20.77
     ATOM   451 CB  THR A  61  0   6.245 48.170 13.535 1.00 22.69
  5  ATOM   452 OG1 THR A  61  0   6.668 46.918 14.096 1.00 23.55
     ATOM   453 CG2 THR A  61  0   7.444 48.976 13.119 1.00 20.92
     ATOM   454 N   SER A  62  0   6.702 48.449 16.507 1.00 22.38
     ATOM   455 CA  SER A  62  0   7.599 48.672 17.633 1.00 22.47
     ATOM   456 C   SER A  62  0   8.381 47.380 17.893 1.00 22.12
 10  ATOM   457 O   SER A  62  0   7.763 46.331 18.124 1.00 20.53
     ATOM   458 CB  SER A  62  0   6.784 49.033 18.882 1.00 22.02
     ATOM   459 OG  SER A  62  0   7.666 49.570 19.832 1.00 21.19
     ATOM   460 N   ILE A  63  0   9.716 47.451 17.806 1.00 21.17
     ATOM   461 CA  ILE A  63  0  10.513 46.240 17.960 1.00 18.32
 15  ATOM   462 C   ILE A  63  0  11.095 46.034 19.354 1.00 18.28
     ATOM   463 O   ILE A  63  0  11.832 46.909 19.826 1.00 19.63
     ATOM   464 CB  ILE A  63  0  11.642 46.234 16.924 1.00 16.68
     ATOM   465 CG1 ILE A  63  0  11.166 46.509 15.508 1.00 18.51
     ATOM   466 CG2 ILE A  63  0  12.319 44.848 16.906 1.00 16.78
 20  ATOM   467 CD1 ILE A  63  0  10.055 45.625 14.994 1.00 18.25
     ATOM   468 N   HIS A  64  0  10.880 44.890 19.985 1.00 15.18
     ATOM   469 CA  HIS A  64  0  11.478 44.539 21.261 1.00 15.51
     ATOM   470 C   HIS A  64  0  12.648 43.559 21.029 1.00 16.73
     ATOM   471 O   HIS A  64  0  12.491 42.591 20.279 1.00 16.85
 25  ATOM   472 CB  HIS A  64  0  10.512 43.912 22.239 1.00 14.37
     ATOM   473 CG  HIS A  64  0  11.033 43.420 23.546 1.00 14.47
     ATOM   474 ND1 HIS A  64  0  11.763 44.191 24.410 1.00 12.89
     ATOM   475 CD2 HIS A  64  0  10.883 42.223 24.193 1.00 14.85
     ATOM   476 CE1 HIS A  64  0  12.067 43.518 25.498 1.00 11.53
 30  ATOM   477 NE2 HIS A  64  0  11.547 42.325 25.423 1.00 13.63
     ATOM   478 N   TRP A  65  0  13.761 43.781 21.723 1.00 14.37
     ATOM   479 CA  TRP A  65  0  14.966 42.926 21.577 1.00 13.92
     ATOM   480 C   TRP A  65  0  14.987 42.084 22.840 1.00 13.50
     ATOM   481 O   TRP A  65  0  15.482 42.538 23.901 1.00 12.84
 35  ATOM   482 CB  TRP A  65  0  16.189 43.825 21.371 1.00 13.50
     ATOM   483 CG  TRP A  65  0  15.890 45.020 20.492 1.00 13.19
     ATOM   484 CD1 TRP A  65  0  15.453 46.247 20.913 1.00 12.42
     ATOM   485 CD2 TRP A  65  0  15.908 45.087 19.068 1.00 13.61
```

```
    ATOM   486 NE1 TRP A 65 0  15.234 47.067 19.862 1.00 11.49
    ATOM   487 CE2 TRP A 65 0  15.511 46.390 18.710 1.00 13.77
    ATOM   488 CE3 TRP A 65 0  16.251 44.174 18.061 1.00 14.35
    ATOM   489 CZ2 TRP A 65 0  15.439 46.815 17.378 1.00 14.99
  5 ATOM   490 CZ3 TRP A 65 0  16.169 44.572 16.735 1.00 13.99
    ATOM   491 CH2 TRP A 65 0  15.756 45.869 16.411 1.00 15.82
    ATOM   492 N   HIS A 66 0  14.295 40.941 22.747 1.00 10.39
    ATOM   493 CA  HIS A 66 0  13.939 40.200 23.966 1.00 12.00
    ATOM   494 C   HIS A 66 0  15.158 39.653 24.698 1.00 11.34
 10 ATOM   495 O   HIS A 66 0  15.889 38.859 24.130 1.00 11.51
    ATOM   496 CB  HIS A 66 0  12.923 39.069 23.629 1.00 10.76
    ATOM   497 CG  HIS A 66 0  12.418 38.308 24.808 1.00 11.26
    ATOM   498 ND1 HIS A 66 0  11.106 38.085 25.092 1.00 13.10
    ATOM   499 CD2 HIS A 66 0  13.050 37.676 25.824 1.00 13.49
 15 ATOM   500 CE1 HIS A 66 0  10.919 37.407 26.191 1.00 12.50
    ATOM   501 NE2 HIS A 66 0  12.116 37.146 26.683 1.00 13.71
    ATOM   502 N   GLY A 67 0  15.345 39.971 25.948 1.00 12.84
    ATOM   503 CA  GLY A 67 0  16.492 39.469 26.719 1.00 13.36
    ATOM   504 C   GLY A 67 0  17.596 40.500 26.914 1.00 13.11
 20 ATOM   505 O   GLY A 67 0  18.435 40.289 27.788 1.00 13.36
    ATOM   506 N   LEU A 68 0  17.641 41.558 26.131 1.00 12.89
    ATOM   507 CA  LEU A 68 0  18.659 42.598 26.300 1.00 15.22
    ATOM   508 C   LEU A 68 0  18.235 43.501 27.448 1.00 16.14
    ATOM   509 O   LEU A 68 0  17.029 43.842 27.505 1.00 16.50
 25 ATOM   510 CB  LEU A 68 0  18.929 43.320 24.988 1.00 15.98
    ATOM   511 CG  LEU A 68 0  20.002 42.638 24.114 1.00 19.57
    ATOM   512 CD1 LEU A 68 0  19.719 41.185 23.809 1.00 20.39
    ATOM   513 CD2 LEU A 68 0  20.188 43.316 22.758 1.00 19.59
    ATOM   514 N   PHE A 69 0  19.125 43.848 28.386 1.00 13.24
 30 ATOM   515 CA  PHE A 69 0  18.700 44.657 29.526 1.00 13.85
    ATOM   516 C   PHE A 69 0  18.499 46.128 29.205 1.00 14.34
    ATOM   517 O   PHE A 69 0  17.806 46.879 29.895 1.00 15.02
    ATOM   518 CB  PHE A 69 0  19.770 44.579 30.637 1.00 16.02
    ATOM   519 CG  PHE A 69 0  20.112 43.187 31.072 1.00 16.45
 35 ATOM   520 CD1 PHE A 69 0  19.172 42.162 31.026 1.00 16.68
    ATOM   521 CD2 PHE A 69 0  21.381 42.927 31.578 1.00 16.78
    ATOM   522 CE1 PHE A 69 0  19.504 40.883 31.448 1.00 18.86
    ATOM   523 CE2 PHE A 69 0  21.717 41.652 32.001 1.00 17.34
```

44

```
      ATOM  524 CZ  PHE A 69 0  20.782 40.628 31.932 1.00 18.09
      ATOM  525 N   GLN A 70 0  19.081 46.611 28.130 1.00 12.22
      ATOM  526 CA  GLN A 70 0  18.919 47.990 27.708 1.00 15.20
      ATOM  527 C   GLN A 70 0  19.242 49.004 28.799 1.00 16.76
   5  ATOM  528 O   GLN A 70 0  18.555 50.016 28.919 1.00 16.08
      ATOM  529 CB  GLN A 70 0  17.488 48.115 27.232 1.00 15.52
     ·ATOM  530 CG  GLN A 70 0  17.168 47.303 26.003 1.00 17.37
      ATOM  531 CD  GLN A 70 0  17.781 47.744 24.709 1.00 17.70
      ATOM  532 OE1 GLN A 70 0  17.557 47.090 23.676 1.00 21.63
  10  ATOM  533 NE2 GLN A 70 0  18.549 48.805 24.620 1.00 16.79
      ATOM  534 N   ARG A 71 0  20.338 48.804 29.518 1.00 16.49
      ATOM  535 CA  ARG A 71 0  20.765 49.712 30.588 1.00 18.41
      ATOM  536 C   ARG A 71 0  21.239 51.011 29.970 1.00 16.23
      ATOM  537 O   ARG A 71 0  22.059 50.998 29.027 1.00 14.48
  15  ATOM  538 CB  ARG A 71 0  21.827 48.942 31.382 1.00 22.65
      ATOM  539 CG  ARG A 71 0  22.273 49.589 32.671 1.00 29.50
      ATOM  540 CD  ARG A 71 0  23.286 48.756 33.457 1.00 32.92
      ATOM  541 NE  ARG A 71 0  22.712 47.550 34.035 1.00 38.11
      ATOM  542 CZ  ARG A 71 0  22.551 46.358 33.452 1.00 40.14
  20  ATOM  543 NH1 ARG A 71 0  22.939 46.138 32.190 1.00 41.23
      ATOM  544 NH2 ARG A 71 0  22.022 45.333 34.130 1.00 40.89
      ATOM  545 N   GLY A 72 0  20.613 52.145 30.311 1.00 14.82
      ATOM  546 CA  GLY A 72 0  20.981 53.414 29.676 1.00 14.51
      ATOM  547 C   GLY A 72 0  20.268 53.606 28.338 1.00 15.55
  25  ATOM  548 O   GLY A 72 0  20.401 54.706 27.777 1.00 16.32
      ATOM  549 N   THR A 73 0  19.503 52.651 27.804 1.00 12.12
      ATOM  550 CA  THR A 73 0  18.857 52.781 26.516 1.00 12.50
      ATOM  551 C   THR A 73 0  17.418 52.252 26.621 1.00 13.98
      ATOM  552 O   THR A 73 0  16.890 51.534 25.776 1.00 13.81
  30  ATOM  553 CB  THR A 73 0  19.577 52.086 25.346 1.00 12.21
      ATOM  554 OG1 THR A 73 0  19.854 50.711 25.666 1.00 12.83
      ATOM  555 CG2 THR A 73 0  20.944 52.711 25.000 1.00  9.81
      ATOM  556 N   ASN A 74 0  16.744 52.617 27.708 1.00 12.97
      ATOM  557 CA  ASN A 74 0  15.354 52.273 27.951 1.00 14.93
  35  ATOM  558 C   ASN A 74 0  14.469 52.718 26.784 1.00 15.92
      ATOM  559 O   ASN A 74 0  13.501 52.030 26.455 1.00 16.56
      ATOM  560 CB  ASN A 74 0  14.851 52.821 29.271 1.00 13.06
      ATOM  561 CG  ASN A 74 0  13.385 52.519 29.556 1.00 15.47
```

```
      ATOM  562 OD1 ASN A 74  0  12.557 53.250 29.021 1.00 13.99
      ATOM  563 ND2 ASN A 74  0  13.063 51.500 30.367 1.00 13.91
      ATOM  564 N   TRP A 75  0  14.806 53.765 26.041 1.00 16.16
      ATOM  565 CA  TRP A 75  0  14.036 54.262 24.917 1.00 16.49
    5 ATOM  566 C   TRP A 75  0  14.050 53.345 23.701 1.00 17.29
      ATOM  567 O   TRP A 75  0  13.235 53.529 22.776 1.00 16.34
      ATOM  568 CB  TRP A 75  0  14.516 55.657 24.509 1.00 15.90
      ATOM  569 CG  TRP A 75  0  15.990 55.705 24.207 1.00 16.04
      ATOM  570 CD1 TRP A 75  0  17.011 55.972 25.072 1.00 14.90
   10 ATOM  571 CD2 TRP A 75  0  16.584 55.475 22.916 1.00 15.94
      ATOM  572 NE1 TRP A 75  0  18.210 55.917 24.384 1.00 15.89
      ATOM  573 CE2 TRP A 75  0  17.977 55.624 23.076 1.00 15.80
      ATOM  574 CE3 TRP A 75  0  16.060 55.171 21.656 1.00 14.88
      ATOM  575 CZ2 TRP A 75  0  18.867 55.459 22.016 1.00 17.60
   15 ATOM  576 CZ3 TRP A 75  0  16.928 55.025 20.603 1.00 16.64
      ATOM  577 CH2 TRP A 75  0  18.321 55.153 20.785 1.00 18.16
      ATOM  578 N   ALA A 76  0  14.962 52.372 23.675 1.00 15.12
      ATOM  579 CA  ALA A 76  0  15.075 51.430 22.578 1.00 14.61
      ATOM  580 C   ALA A 76  0  14.569 50.047 22.971 1.00 13.98
   20 ATOM  581 O   ALA A 76  0  14.617 49.132 22.159 1.00 14.20
      ATOM  582 CB  ALA A 76  0  16.554 51.354 22.157 1.00 13.68
      ATOM  583 N   ASP A 77  0  13.941 49.885 24.121 1.00 14.47
      ATOM  584 CA  ASP A 77  0  13.409 48.605 24.586 1.00 14.23
      ATOM  585 C   ASP A 77  0  12.198 48.167 23.762 1.00 15.04
   25 ATOM  586 O   ASP A 77  0  11.982 46.946 23.638 1.00 13.78
      ATOM  587 CB  ASP A 77  0  13.112 48.567 26.072 1.00 13.41
      ATOM  588 CG  ASP A 77  0  12.945 47.155 26.612 1.00 14.93
      ATOM  589 OD1 ASP A 77  0  11.943 46.986 27.345 1.00 15.07
      ATOM  590 OD2 ASP A 77  0  13.744 46.217 26.334 1.00 13.73
   30 ATOM  591 N   GLY A 78  0  11.458 49.095 23.160 1.00 13.63
      ATOM  592 CA  GLY A 78  0  10.442 48.686 22.210 1.00 14.96
      ATOM  593 C   GLY A 78  0   9.040 48.309 22.631 1.00 16.75
      ATOM  594 O   GLY A 78  0   8.276 47.865 21.755 1.00 16.49
      ATOM  595 N   ALA A 79  0   8.631 48.436 23.886 1.00 15.34
   35 ATOM  596 CA  ALA A 79  0   7.252 48.176 24.270 1.00 14.70
      ATOM  597 C   ALA A 79  0   6.490 49.495 24.084 1.00 17.51
      ATOM  598 O   ALA A 79  0   6.690 50.486 24.807 1.00 17.05
      ATOM  599 CB  ALA A 79  0   7.145 47.701 25.708 1.00 14.78
```

```
   ATOM    600  N   ASP A  80  0    5.641 49.536 23.053  1.00 18.56
   ATOM    601  CA  ASP A  80  0    4.859 50.741 22.798  1.00 19.52
   ATOM    602  C   ASP A  80  0    3.959 50.963 24.010  1.00 17.61
   ATOM    603  O   ASP A  80  0    3.530 49.999 24.664  1.00 16.72
 5 ATOM    604  CB  ASP A  80  0    4.044 50.714 21.510  1.00 24.02
   ATOM    605  CG  ASP A  80  0    3.003 49.607 21.549  1.00 28.13
   ATOM    606  OD1 ASP A  80  0    3.410 48.417 21.541  1.00 30.66
   ATOM    607  OD2 ASP A  80  0    1.803 49.959 21.603  1.00 30.61
   ATOM    608  N   GLY A  81  0    3.776 52.242 24.337  1.00 15.85
10 ATOM    609  CA  GLY A  81  0    2.991 52.566 25.532  1.00 16.27
   ATOM    610  C   GLY A  81  0    3.846 52.615 26.784  1.00 18.72
   ATOM    611  O   GLY A  81  0    3.405 52.983 27.890  1.00 20.61
   ATOM    612  N   VAL A  82  0    5.108 52.173 26.725  1.00 19.11
   ATOM    613  CA  VAL A  82  0    5.978 52.119 27.890  1.00 19.14
15 ATOM    614  C   VAL A  82  0    7.288 52.851 27.590  1.00 18.41
   ATOM    615  O   VAL A  82  0    7.594 53.839 28.242  1.00 16.79
   ATOM    616  CB  VAL A  82  0    6.266 50.697 28.390  1.00 19.82
   ATOM    617  CG1 VAL A  82  0    7.059 50.741 29.710  1.00 21.37
   ATOM    618  CG2 VAL A  82  0    4.995 49.894 28.640  1.00 19.27
20 ATOM    619  N   ASN A  83  0    7.982 52.408 26.551  1.00 17.90
   ATOM    620  CA  ASN A  83  0    9.271 52.926 26.147  1.00 16.94
   ATOM    621  C   ASN A  83  0    9.226 53.778 24.886  1.00 18.32
   ATOM    622  O   ASN A  83  0   10.175 54.551 24.634  1.00 20.58
   ATOM    623  CB  ASN A  83  0   10.249 51.747 25.937  1.00 15.23
25 ATOM    624  CG  ASN A  83  0   10.112 50.745 27.063  1.00 16.00
   ATOM    625  OD1 ASN A  83  0    9.493 49.676 26.879  1.00 14.98
   ATOM    626  ND2 ASN A  83  0   10.583 51.131 28.249  1.00 13.17
   ATOM    627  N   GLN A  84  0    8.183 53.668 24.066  1.00 16.40
   ATOM    628  CA  GLN A  84  0    8.080 54.464 22.867  1.00 16.34
30 ATOM    629  C   GLN A  84  0    6.658 54.465 22.309  1.00 17.95
   ATOM    630  O   GLN A  84  0    5.816 53.679 22.728  1.00 17.69
   ATOM    631  CB  GLN A  84  0    8.995 53.953 21.754  1.00 17.98
   ATOM    632  CG  GLN A  84  0    8.456 52.654 21.127  1.00 16.63
   ATOM    633  CD  GLN A  84  0    9.272 52.225 19.938  1.00 18.17
35 ATOM    634  OE1 GLN A  84  0    8.994 52.601 18.792  1.00 20.91
   ATOM    635  NE2 GLN A  84  0   10.279 51.385 20.096  1.00 18.70
   ATOM    636  N   CYS A  85  0    6.419 55.350 21.365  1.00 18.60
   ATOM    637  CA  CYS A  85  0    5.140 55.344 20.622  1.00 20.25
```

```
      ATOM   638  C   CYS A 85  0   5.512 54.555 19.375 1.00 19.55
      ATOM   639  O   CYS A 85  0   6.690 54.546 18.995 1.00 18.92
      ATOM   640  CB  CYS A 85  0   4.772 56.786 20.228 1.00 22.20
      ATOM   641  SG  CYS A 85  0   3.899 57.783 21.481 1.00 24.65
 5    ATOM   642  N   PRO A 86  0   4.589 53.951 18.674 1.00 21.19
      ATOM   643  CA  PRO A 86  0   4.869 53.152 17.498 1.00 20.78
      ATOM   644  C   PRO A 86  0   5.560 53.930 16.394 1.00 21.46
      ATOM   645  O   PRO A 86  0   5.453 55.137 16.298 1.00 23.08
      ATOM   646  CB  PRO A 86  0   3.530 52.555 17.028 1.00 19.94
 10   ATOM   647  CG  PRO A 86  0   2.667 52.720 18.252 1.00 19.59
      ATOM   648  CD  PRO A 86  0   3.174 53.872 19.062 1.00 20.46
      ATOM   649  N   ILE A 87  0   6.318 53.259 15.550 1.00 20.95
      ATOM   650  CA  ILE A 87  0   6.907 53.773 14.337 1.00 22.43
      ATOM   651  C   ILE A 87  0   5.768 53.641 13.292 1.00 22.80
 15   ATOM   652  O   ILE A 87  0   5.148 52.562 13.228 1.00 21.61
      ATOM   653  CB  ILE A 87  0   8.105 52.954 13.844 1.00 21.99
      ATOM   654  CG1 ILE A 87  0   9.130 52.696 14.944 1.00 24.18
      ATOM   655  CG2 ILE A 87  0   8.773 53.656 12.674 1.00 22.91
      ATOM   656  CD1 ILE A 87  0  10.256 51.776 14.514 1.00 23.87
 20   ATOM   657  N   SER A 88  0   5.464 54.702 12.570 1.00 22.64
      ATOM   658  CA  SER A 88  0   4.338 54.709 11.647 1.00 22.85
      ATOM   659  C   SER A 88  0   4.751 54.268 10.249 1.00 23.35
      ATOM   660  O   SER A 88  0   5.870 54.489  9.764 1.00 23.30
      ATOM   661  CB  SER A 88  0   3.767 56.137 11.518 1.00 24.00
 25   ATOM   662  OG  SER A 88  0   3.379 56.770 12.720 1.00 23.93
      ATOM   663  N   PRO A 89  0   3.778 53.752  9.514 1.00 23.60
      ATOM   664  CA  PRO A 89  0   3.955 53.382  8.116 1.00 25.19
      ATOM   665  C   PRO A 89  0   4.579 54.556  7.361 1.00 26.58
      ATOM   666  O   PRO A 89  0   4.177 55.699  7.585 1.00 26.66
 30   ATOM   667  CB  PRO A 89  0   2.566 53.065  7.555 1.00 23.59
      ATOM   668  CG  PRO A 89  0   1.740 52.856  8.798 1.00 22.37
      ATOM   669  CD  PRO A 89  0   2.415 53.513  9.970 1.00 23.25
      ATOM   670  N   GLY A 90  0   5.588 54.311  6.550 1.00 27.73
      ATOM   671  CA  GLY A 90  0   6.223 55.338  5.748 1.00 30.55
 35   ATOM   672  C   GLY A 90  0   7.384 56.032  6.438 1.00 32.38
      ATOM   673  O   GLY A 90  0   8.050 56.894  5.879 1.00 32.53
      ATOM   674  N   HIS A 91  0   7.639 55.693  7.702 1.00 32.77
      ATOM   675  CA  HIS A 91  0   8.691 56.283  8.494 1.00 32.55
```

```
     ATOM   676 C   HIS A 91 0    9.649 55.179  8.982 1.00 32.36
     ATOM   677 O   HIS A 91 0    9.381 53.972  8.961 1.00 31.30
     ATOM   678 CB  HIS A 91 0    8.118 57.016  9.722 1.00 33.75
     ATOM   679 CG  HIS A 91 0    7.147 58.073  9.295 1.00 34.64
  5  ATOM   680 ND1 HIS A 91 0    7.519 59.381  9.072 1.00 34.41
     ATOM   681 CD2 HIS A 91 0    5.822 57.977  9.002 1.00 34.89
     ATOM   682 CE1 HIS A 91 0    6.450 60.050  8.679 1.00 34.87
     ATOM   683 NE2 HIS A 91 0    5.410 59.233  8.628 1.00 35.14
     ATOM   684 N   ALA A 92 0   10.786 55.668  9.437 1.00 29.57
 10  ATOM   685 CA  ALA A 92 0   11.895 54.898  9.937 1.00 27.71
     ATOM   686 C   ALA A 92 0   12.316 55.347 11.337 1.00 27.41
     ATOM   687 O   ALA A 92 0   12.076 56.484 11.741 1.00 26.12
     ATOM   688 CB  ALA A 92 0   13.051 55.057  8.967 1.00 25.23
     ATOM   689 N   PHE A 93 0   12.931 54.418 12.081 1.00 26.87
 15  ATOM   690 CA  PHE A 93 0   13.441 54.760 13.405 1.00 25.87
     ATOM   691 C   PHE A 93 0   14.746 54.008 13.632 1.00 25.21
     ATOM   692 O   PHE A 93 0   14.797 52.810 13.347 1.00 25.80
     ATOM   693 CB  PHE A 93 0   12.457 54.456 14.526 1.00 25.30
     ATOM   694 CG  PHE A 93 0   12.964 54.955 15.847 1.00 25.41
 20  ATOM   695 CD1 PHE A 93 0   13.154 56.309 16.061 1.00 25.36
     ATOM   696 CD2 PHE A 93 0   13.276 54.057 16.853 1.00 25.31
     ATOM   697 CE1 PHE A 93 0   13.637 56.753 17.285 1.00 26.54
     ATOM   698 CE2 PHE A 93 0   13.754 54.503 18.078 1.00 25.39
     ATOM   699 CZ  PHE A 93 0   13.935 55.857 18.302 1.00 25.01
 25  ATOM   700 N   LEU A 94 0   15.756 54.699 14.136 1.00 23.39
     ATOM   701 CA  LEU A 94 0   17.046 54.058 14.361 1.00 23.35
     ATOM   702 C   LEU A 94 0   17.191 53.611 15.804 1.00 23.22
     ATOM   703 O   LEU A 94 0   17.261 54.431 16.714 1.00 23.47
     ATOM   704 CB  LEU A 94 0   18.186 54.994 13.943 1.00 24.96
 30  ATOM   705 CG  LEU A 94 0   19.630 54.555 14.170 1.00 26.28
     ATOM   706 CD1 LEU A 94 0   19.979 53.313 13.352 1.00 25.99
     ATOM   707 CD2 LEU A 94 0   20.627 55.678 13.887 1.00 26.06
     ATOM   708 N   TYR A 95 0   17.261 52.293 16.023 1.00 21.81
     ATOM   709 CA  TYR A 95 0   17.481 51.780 17.379 1.00 19.72
 35  ATOM   710 C   TYR A 95 0   18.991 51.663 17.585 1.00 20.90
     ATOM   711 O   TYR A 95 0   19.690 51.248 16.656 1.00 20.74
     ATOM   712 CB  TYR A 95 0   16.831 50.448 17.609 1.00 17.86
     ATOM   713 CG  TYR A 95 0   15.329 50.411 17.691 1.00 16.35
```

```
      ATOM   714 CD1 TYR A 95 0   14.541 50.288 16.535 1.00 16.89
      ATOM   715 CD2 TYR A 95 0   14.701 50.442 18.911 1.00 15.71
      ATOM   716 CE1 TYR A 95 0   13.157 50.205 16.621 1.00 17.21
      ATOM   717 CE2 TYR A 95 0   13.325 50.362 19.033 1.00 16.25
  5   ATOM   718 CZ  TYR A 95 0   12.568 50.266 17.874 1.00 17.97
      ATOM   719 OH  TYR A 95 0   11.205 50.189 18.001 1.00 18.61
      ATOM   720 N   LYS A 96 0   19.475 52.105 18.752 1.00 20.56
      ATOM   721 CA  LYS A 96 0   20.917 52.058 18.975 1.00 21.77
      ATOM   722 C   LYS A 96 0   21.139 51.519 20.386 1.00 20.91
 10   ATOM   723 O   LYS A 96 0   20.558 52.122 21.286 1.00 21.98
      ATOM   724 CB  LYS A 96 0   21.565 53.427 18.960 1.00 22.89
      ATOM   725 CG  LYS A 96 0   21.857 54.046 17.609 1.00 26.39
      ATOM   726 CD  LYS A 96 0   22.749 55.251 17.923 1.00 30.80
      ATOM   727 CE  LYS A 96 0   22.732 56.348 16.884 1.00 32.90
 15   ATOM   728 NZ  LYS A 96 0   23.767 57.378 17.277 1.00 36.06
      ATOM   729 N   PHE A 97 0   21.871 50.437 20.520 1.00 18.14
      ATOM   730 CA  PHE A 97 0   22.062 49.863 21.854 1.00 18.19
      ATOM   731 C   PHE A 97 0   23.276 48.928 21.805 1.00 16.76
      ATOM   732 O   PHE A 97 0   23.870 48.700 20.747 1.00 14.19
 20   ATOM   733 CB  PHE A 97 0   20.816 49.067 22.307 1.00 17.34
      ATOM   734 CG  PHE A 97 0   20.379 48.026 21.304 1.00 17.56
      ATOM   735 CD1 PHE A 97 0   20.873 46.732 21.348 1.00 16.27
      ATOM   736 CD2 PHE A 97 0   19.451 48.343 20.326 1.00 18.65
      ATOM   737 CE1 PHE A 97 0   20.476 45.801 20.398 1.00 17.76
 25   ATOM   738 CE2 PHE A 97 0   19.026 47.408 19.386 1.00 18.64
      ATOM   739 CZ  PHE A 97 0   19.546 46.120 19.416 1.00 17.55
      ATOM   740 N   THR A 98 0   23.552 48.348 22.971 1.00 17.45
      ATOM   741 CA  THR A 98 0   24.644 47.359 22.992 1.00 17.00
      ATOM   742 C   THR A 98 0   24.304 46.333 24.042 1.00 16.63
 30   ATOM   743 O   THR A 98 0   23.725 46.631 25.090 1.00 15.86
      ATOM   744 CB  THR A 98 0   26.028 47.990 23.256 1.00 17.53
      ATOM   745 OG1 THR A 98 0   27.017 46.924 23.372 1.00 19.01
      ATOM   746 CG2 THR A 98 0   26.088 48.807 24.525 1.00 14.85
      ATOM   747 N   PRO A 99 0   24.740 45.097 23.831 1.00 15.98
 35   ATOM   748 CA  PRO A 99 0   24.601 44.019 24.787 1.00 15.11
      ATOM   749 C   PRO A 99 0   25.445 44.270 26.020 1.00 15.99
      ATOM   750 O   PRO A 99 0   25.260 43.633 27.064 1.00 15.94
      ATOM   751 CB  PRO A 99 0   25.025 42.717 24.098 1.00 15.83
```

```
   ATOM   752 CG  PRO A 99  0  25.042 43.140 22.644 1.00 17.12
   ATOM   753 CD  PRO A 99  0  25.362 44.627 22.601 1.00 15.68
   ATOM   754 N   ALA A 100 0  26.452 45.149 25.932 1.00 17.29
   ATOM   755 CA  ALA A 100 0  27.316 45.501 27.050 1.00 16.88
 5 ATOM   756 C   ALA A 100 0  27.919 44.293 27.754 1.00 16.16
   ATOM   757 O   ALA A 100 0  27.779 44.187 28.977 1.00 18.13
   ATOM   758 CB  ALA A 100 0  26.498 46.292 28.084 1.00 14.96
   ATOM   759 N   GLY A 101 0  28.474 43.360 27.033 1.00 16.41
   ATOM   760 CA  GLY A 101 0  29.063 42.172 27.599 1.00 17.49
10 ATOM   761 C   GLY A 101 0  28.130 40.994 27.769 1.00 16.15
   ATOM   762 O   GLY A 101 0  28.593 39.930 28.137 1.00 16.57
   ATOM   763 N   HIS A 102 0  26.838 41.120 27.521 1.00 17.58
   ATOM   764 CA  HIS A 102 0  25.858 40.058 27.804 1.00 15.77
   ATOM   765 C   HIS A 102 0  25.707 39.165 26.600 1.00 15.28
15 ATOM   766 O   HIS A 102 0  25.087 39.641 25.662 1.00 17.64
   ATOM   767 CB  HIS A 102 0  24.498 40.666 28.186 1.00 17.95
   ATOM   768 CG  HIS A 102 0  23.432 39.661 28.493 1.00 20.00
   ATOM   769 ND1 HIS A 102 0  22.099 40.005 28.547 1.00 20.59
   ATOM   770 CD2 HIS A 102 0  23.475 38.323 28.772 1.00 20.09
20 ATOM   771 CE1 HIS A 102 0  21.398 38.937 28.866 1.00 20.77
   ATOM   772 NE2 HIS A 102 0  22.201 37.896 29.016 1.00 20.56
   ATOM   773 N   ALA A 103 0  26.277 37.958 26.584 1.00 13.32
   ATOM   774 CA  ALA A 103 0  26.141 37.127 25.415 1.00 13.99
   ATOM   775 C   ALA A 103 0  24.974 36.156 25.649 1.00 13.43
25 ATOM   776 O   ALA A 103 0  24.571 35.905 26.784 1.00 11.81
   ATOM   777 CB  ALA A 103 0  27.418 36.329 25.151 1.00 16.36
   ATOM   778 N   GLY A 104 0  24.459 35.610 24.554 1.00 12.38
   ATOM   779 CA  GLY A 104 0  23.381 34.632 24.778 1.00 12.85
   ATOM   780 C   GLY A 104 0  22.480 34.451 23.581 1.00 11.06
30 ATOM   781 O   GLY A 104 0  22.674 35.057 22.515 1.00 10.91
   ATOM   782 N   THR A 105 0  21.442 33.650 23.794 1.00 10.14
   ATOM   783 CA  THR A 105 0  20.490 33.394 22.704 1.00 10.04
   ATOM   784 C   THR A 105 0  19.238 34.236 22.989 1.00  9.52
   ATOM   785 O   THR A 105 0  18.738 34.194 24.125 1.00  7.52
35 ATOM   786 CB  THR A 105 0  20.114 31.913 22.665 1.00 12.67
   ATOM   787 OG1 THR A 105 0  21.273 31.075 22.593 1.00 13.47
   ATOM   788 CG2 THR A 105 0  19.187 31.684 21.468 1.00 12.75
   ATOM   789 N   PHE A 106 0  18.842 35.065 22.044 1.00  7.76
```

```
    ATOM   790  CA  PHE A 106 0   17.731  35.992  22.243  1.00 10.15
    ATOM   791  C   PHE A 106 0   16.756  35.910  21.068  1.00  8.42
    ATOM   792  O   PHE A 106 0   16.941  35.083  20.166  1.00  8.33
    ATOM   793  CB  PHE A 106 0   18.283  37.460  22.369  1.00 10.19
  5 ATOM   794  CG  PHE A 106 0   19.291  37.577  23.506  1.00 12.95
    ATOM   795  CD1 PHE A 106 0   18.905  37.443  24.815  1.00 11.44
    ATOM   796  CD2 PHE A 106 0   20.654  37.775  23.230  1.00 12.37
    ATOM   797  CE1 PHE A 106 0   19.855  37.531  25.822  1.00 14.20
    ATOM   798  CE2 PHE A 106 0   21.574  37.857  24.273  1.00 11.56
 10 ATOM   799  CZ  PHE A 106 0   21.202  37.733  25.599  1.00  9.45
    ATOM   800  N   TRP A 107 0   15.869  36.887  20.917  1.00  6.61
    ATOM   801  CA  TRP A 107 0   15.062  36.977  19.713  1.00 10.20
    ATOM   802  C   TRP A 107 0   14.511  38.398  19.625  1.00 10.63
    ATOM   803  O   TRP A 107 0   14.463  39.036  20.657  1.00 13.71
 15 ATOM   804  CB  TRP A 107 0   13.928  35.966  19.636  1.00  7.49
    ATOM   805  CG  TRP A 107 0   12.945  35.916  20.755  1.00  9.41
    ATOM   806  CD1 TRP A 107 0   13.136  35.804  22.106  1.00 10.53
    ATOM   807  CD2 TRP A 107 0   11.509  36.004  20.581  1.00  9.17
    ATOM   808  NE1 TRP A 107 0   11.929  35.784  22.768  1.00 10.63
 20 ATOM   809  CE2 TRP A 107 0   10.924  35.926  21.842  1.00  9.90
    ATOM   810  CE3 TRP A 107 0   10.698  36.144  19.444  1.00  8.77
    ATOM   811  CZ2 TRP A 107 0    9.538  35.947  22.025  1.00 10.01
    ATOM   812  CZ3 TRP A 107 0    9.336  36.167  19.613  1.00  8.60
    ATOM   813  CH2 TRP A 107 0    8.774  36.061  20.890  1.00 10.09
 25 ATOM   814  N   TYR A 108 0   14.117  38.847  18.464  1.00 10.72
    ATOM   815  CA  TYR A 108 0   13.498  40.148  18.302  1.00 12.19
    ATOM   816  C   TYR A 108 0   12.030  39.869  17.875  1.00 13.62
    ATOM   817  O   TYR A 108 0   11.752  38.837  17.245  1.00 13.85
    ATOM   818  CB  TYR A 108 0   14.182  40.994  17.259  1.00 11.05
 30 ATOM   819  CG  TYR A 108 0   14.176  40.413  15.857  1.00 13.89
    ATOM   820  CD1 TYR A 108 0   15.087  39.464  15.423  1.00 12.99
    ATOM   821  CD2 TYR A 108 0   13.257  40.897  14.920  1.00 14.94
    ATOM   822  CE1 TYR A 108 0   15.064  38.979  14.130  1.00 13.64
    ATOM   823  CE2 TYR A 108 0   13.216  40.409  13.624  1.00 15.34
 35 ATOM   824  CZ  TYR A 108 0   14.123  39.443  13.236  1.00 14.99
    ATOM   825  OH  TYR A 108 0   14.063  38.960  11.946  1.00 16.68
    ATOM   826  N   HIS A 109 0   11.123  40.752  18.254  1.00 12.81
    ATOM   827  CA  HIS A 109 0    9.735  40.630  17.826  1.00 14.92
```

ATOM 828 C HIS A 109 0 9.057 41.988 17.991 1.00 15.96
ATOM 829 O HIS A 109 0 9.392 42.800 18.875 1.00 15.67
ATOM 830 CB HIS A 109 0 8.903 39.566 18.550 1.00 12.30
ATOM 831 CG HIS A 109 0 8.804 39.727 20.036 1.00 12.30
5 ATOM 832 ND1 HIS A 109 0 7.788 40.429 20.666 1.00 9.89
ATOM 833 CD2 HIS A 109 0 9.614 39.264 21.034 1.00 10.76
ATOM 834 CE1 HIS A 109 0 7.982 40.379 21.971 1.00 8.49
ATOM 835 NE2 HIS A 109 0 9.086 39.679 22.224 1.00 7.92
ATOM 836 N SER A 110 0 8.070 42.203 17.122 1.00 16.26
10 ATOM 837 CA SER A 110 0 7.244 43.404 17.300 1.00 14.55
ATOM 838 C SER A 110 0 6.548 43.283 18.646 1.00 13.56
ATOM 839 O SER A 110 0 6.219 42.191 19.140 1.00 13.54
ATOM 840 CB SER A 110 0 6.219 43.543 16.159 1.00 16.69
ATOM 841 OG SER A 110 0 5.212 44.481 16.508 1.00 15.32
15 ATOM 842 N HIS A 111 0 6.396 44.395 19.359 1.00 14.60
ATOM 843 CA HIS A 111 0 5.724 44.397 20.645 1.00 16.23
ATOM 844 C HIS A 111 0 4.349 45.070 20.478 1.00 18.61
ATOM 845 O HIS A 111 0 3.713 45.391 21.473 1.00 21.72
ATOM 846 CB HIS A 111 0 6.478 45.166 21.721 1.00 14.37
20 ATOM 847 CG HIS A 111 0 6.392 44.519 23.077 1.00 15.33
ATOM 848 ND1 HIS A 111 0 5.341 44.660 23.947 1.00 14.55
ATOM 849 CD2 HIS A 111 0 7.265 43.676 23.680 1.00 14.72
ATOM 850 CE1 HIS A 111 0 5.589 43.936 25.040 1.00 16.29
ATOM 851 NE2 HIS A 111 0 6.773 43.326 24.920 1.00 15.35
25 ATOM 852 N PHE A 112 0 3.950 45.382 19.258 1.00 18.67
ATOM 853 CA PHE A 112 0 2.725 46.139 19.037 1.00 19.61
ATOM 854 C PHE A 112 0 1.540 45.219 18.777 1.00 19.06
ATOM 855 O PHE A 112 0 1.521 44.630 17.707 1.00 17.50
ATOM 856 CB PHE A 112 0 2.971 47.113 17.875 1.00 21.16
30 ATOM 857 CG PHE A 112 0 1.798 48.019 17.611 1.00 23.12
ATOM 858 CD1 PHE A 112 0 1.456 49.007 18.509 1.00 24.59
ATOM 859 CD2 PHE A 112 0 1.034 47.886 16.466 1.00 24.82
ATOM 860 CE1 PHE A 112 0 0.387 49.852 18.312 1.00 24.29
ATOM 861 CE2 PHE A 112 0 -0.063 48.714 16.243 1.00 25.87
35 ATOM 862 CZ PHE A 112 0 -0.378 49.698 17.161 1.00 25.17
ATOM 863 N GLY A 113 0 0.599 45.092 19.707 1.00 18.05
ATOM 864 CA GLY A 113 0 -0.554 44.236 19.433 1.00 19.69
ATOM 865 C GLY A 113 0 -0.085 42.819 19.096 1.00 22.25

```
     ATOM  866 O   GLY A 113 0    0.937 42.333 19.593 1.00 20.55
     ATOM  867 N   THR A 114 0   -0.817 42.173 18.186 1.00 20.91
     ATOM  868 CA  THR A 114 0   -0.493 40.816 17.749 1.00 20.85
     ATOM  869 C   THR A 114 0    0.296 40.774 16.471 1.00 18.04
  5  ATOM  870 O   THR A 114 0    0.243 39.783 15.743 1.00 18.26
     ATOM  871 CB  THR A 114 0   -1.847 40.095 17.487 1.00 23.93
     ATOM  872 OG1 THR A 114 0   -2.609 40.910 16.554 1.00 25.68
     ATOM  873 CG2 THR A 114 0   -2.571 39.928 18.792 1.00 23.72
     ATOM  874 N   GLN A 115 0    1.023 41.819 16.095 1.00 17.04
 10  ATOM  875 CA  GLN A 115 0    1.792 41.842 14.853 1.00 16.88
     ATOM  876 C   GLN A 115 0    2.881 40.775 14.744 1.00 17.94
     ATOM  877 O   GLN A 115 0    3.203 40.263 13.649 1.00 17.18
     ATOM  878 CB  GLN A 115 0    2.391 43.244 14.757 1.00 17.55
     ATOM  879 CG  GLN A 115 0    3.026 43.601 13.418 1.00 17.65
 15  ATOM  880 CD  GLN A 115 0    3.558 45.024 13.418 1.00 17.73
     ATOM  881 OE1 GLN A 115 0    3.257 45.782 12.482 1.00 19.19
     ATOM  882 NE2 GLN A 115 0    4.334 45.421 14.422 1.00 14.70
     ATOM  883 N   TYR A 116 0    3.515 40.416 15.881 1.00 16.32
     ATOM  884 CA  TYR A 116 0    4.561 39.386 15.859 1.00 15.92
 20  ATOM  885 C   TYR A 116 0    3.935 38.042 15.479 1.00 17.17
     ATOM  886 O   TYR A 116 0    4.584 37.258 14.786 1.00 16.70
     ATOM  887 CB  TYR A 116 0    5.411 39.312 17.096 1.00 13.45
     ATOM  888 CG  TYR A 116 0    5.209 38.487 18.314 1.00 10.97
     ATOM  889 CD1 TYR A 116 0    5.581 37.146 18.394 1.00 11.02
 25  ATOM  890 CD2 TYR A 116 0    4.665 39.052 19.460 1.00 12.18
     ATOM  891 CE1 TYR A 116 0    5.364 36.399 19.532 1.00 10.02
     ATOM  892 CE2 TYR A 116 0    4.491 38.345 20.642 1.00 12.25
     ATOM  893 CZ  TYR A 116 0    4.838 36.996 20.649 1.00 11.73
     ATOM  894 OH  TYR A 116 0    4.642 36.295 21.821 1.00 12.72
 30  ATOM  895 N   CYS A 117 0    2.654 37.829 15.842 1.00 17.70
     ATOM  896 CA  CYS A 117 0    1.965 36.617 15.424 1.00 18.01
     ATOM  897 C   CYS A 117 0    1.883 36.496 13.911 1.00 17.55
     ATOM  898 O   CYS A 117 0    1.796 35.352 13.450 1.00 17.50
     ATOM  899 CB  CYS A 117 0    0.565 36.528 16.042 1.00 17.90
 35  ATOM  900 SG  CYS A 117 0    0.463 36.895 17.810 1.00 19.72
     ATOM  901 N   ASP A 118 0    2.001 37.568 13.136 1.00 15.51
     ATOM  902 CA  ASP A 118 0    1.953 37.509 11.696 1.00 17.74
     ATOM  903 C   ASP A 118 0    3.341 37.445 11.061 1.00 18.72
```

```
   ATOM   904 O   ASP A 118 0    3.494 37.770  9.865 1.00 17.47
   ATOM   905 CB  ASP A 118 0    1.142 38.696 11.131 1.00 18.61
   ATOM   906 CG  ASP A 118 0   -0.356 38.448 11.378 1.00 21.44
   ATOM   907 OD1 ASP A 118 0   -0.826 37.331 11.082 1.00 21.55
 5 ATOM   908 OD2 ASP A 118 0   -1.064 39.333 11.885 1.00 21.54
   ATOM   909 N   GLY A 119 0    4.355 37.095 11.882 1.00 18.19
   ATOM   910 CA  GLY A 119 0    5.671 36.889 11.313 1.00 19.00
   ATOM   911 C   GLY A 119 0    6.751 37.898 11.590 1.00 19.79
   ATOM   912 O   GLY A 119 0    7.909 37.640 11.213 1.00 19.97
10 ATOM   913 N   LEU A 120 0    6.445 39.011 12.280 1.00 18.24
   ATOM   914 CA  LEU A 120 0    7.484 39.991 12.569 1.00 16.08
   ATOM   915 C   LEU A 120 0    8.210 39.565 13.848 1.00 16.53
   ATOM   916 O   LEU A 120 0    7.933 40.051 14.939 1.00 15.31
   ATOM   917 CB  LEU A 120 0    6.918 41.389 12.654 1.00 16.22
15 ATOM   918 CG  LEU A 120 0    7.916 42.540 12.830 1.00 17.73
   ATOM   919 CD1 LEU A 120 0    9.188 42.293 12.043 1.00 17.73
   ATOM   920 CD2 LEU A 120 0    7.302 43.880 12.448 1.00 16.66
   ATOM   921 N   ARG A 121 0    9.144 38.622 13.682 1.00 14.23
   ATOM   922 CA  ARG A 121 0    9.859 37.985 14.773 1.00 14.19
20 ATOM   923 C   ARG A 121 0   11.007 37.152 14.159 1.00 14.09
   ATOM   924 O   ARG A 121 0   10.936 36.787 12.978 1.00 13.72
   ATOM   925 CB  ARG A 121 0    8.934 37.061 15.581 1.00 12.30
   ATOM   926 CG  ARG A 121 0    8.253 35.999 14.728 1.00 12.44
   ATOM   927 CD  ARG A 121 0    7.303 35.098 15.518 1.00 11.94
25 ATOM   928 NE  ARG A 121 0    6.507 34.269 14.604 1.00 12.92
   ATOM   929 CZ  ARG A 121 0    5.413 33.570 14.933 1.00 10.55
   ATOM   930 NH1 ARG A 121 0    4.897 33.483 16.137 1.00  8.12
   ATOM   931 NH2 ARG A 121 0    4.803 32.946 13.930 1.00 10.40
   ATOM   932 N   GLY A 122 0   12.045 36.848 14.937 1.00 12.29
30 ATOM   933 CA  GLY A 122 0   13.162 36.078 14.364 1.00 11.42
   ATOM   934 C   GLY A 122 0   14.185 35.918 15.486 1.00 12.42
   ATOM   935 O   GLY A 122 0   14.095 36.604 16.509 1.00 11.47
   ATOM   936 N   PRO A 123 0   15.164 35.075 15.246 1.00 11.82
   ATOM   937 CA  PRO A 123 0   16.226 34.778 16.190 1.00 12.81
35 ATOM   938 C   PRO A 123 0   17.288 35.857 16.258 1.00 12.41
   ATOM   939 O   PRO A 123 0   17.565 36.580 15.302 1.00 12.03
   ATOM   940 CB  PRO A 123 0   16.833 33.416 15.713 1.00 12.34
   ATOM   941 CG  PRO A 123 0   16.567 33.494 14.223 1.00 12.19
```

```
   ATOM   942 CD  PRO A 123 0   15.283 34.289 14.021 1.00 11.35
   ATOM   943 N   MET A 124 0   17.903 36.027 17.431 1.00 14.30
   ATOM   944 CA  MET A 124 0   18.959 37.024 17.628 1.00 14.19
   ATOM   945 C   MET A 124 0   20.040 36.414 18.528 1.00 15.37
 5 ATOM   946 O   MET A 124 0   19.788 36.067 19.690 1.00 15.41
   ATOM   947 CB  MET A 124 0   18.411 38.290 18.242 1.00 15.94
   ATOM   948 CG  MET A 124 0   19.464 39.345 18.604 1.00 19.30
   ATOM   949 SD  MET A 124 0   18.646 40.875 19.164 1.00 21.94
   ATOM   950 CE  MET A 124 0   19.918 42.061 18.729 1.00 23.64
10 ATOM   951 N   VAL A 125 0   21.212 36.178 17.939 1.00 13.74
   ATOM   952 CA  VAL A 125 0   22.282 35.479 18.658 1.00 13.87
   ATOM   953 C   VAL A 125 0   23.478 36.390 18.872 1.00 13.68
   ATOM   954 O   VAL A 125 0   24.004 36.976 17.945 1.00 14.01
   ATOM   955 CB  VAL A 125 0   22.672 34.139 18.005 1.00 12.58
15 ATOM   956 CG1 VAL A 125 0   23.787 33.383 18.749 1.00 11.23
   ATOM   957 CG2 VAL A 125 0   21.448 33.212 18.033 1.00 12.14
   ATOM   958 N   ILE A 126 0   23.860 36.535 20.135 1.00 14.48
   ATOM   959 CA  ILE A 126 0   25.016 37.295 20.557 1.00 14.53
   ATOM   960 C   ILE A 126 0   26.131 36.348 21.054 1.00 13.58
20 ATOM   961 O   ILE A 126 0   26.061 35.791 22.154 1.00 12.93
   ATOM   962 CB  ILE A 126 0   24.649 38.295 21.662 1.00 14.95
   ATOM   963 CG1 ILE A 126 0   23.563 39.302 21.254 1.00 15.29
   ATOM   964 CG2 ILE A 126 0   25.901 39.014 22.174 1.00 14.24
   ATOM   965 CD1 ILE A 126 0   23.703 39.905 19.896 1.00 15.84
25 ATOM   966 N   TYR A 127 0   27.142 36.146 20.236 1.00 13.66
   ATOM   967 CA  TYR A 127 0   28.278 35.258 20.529 1.00 14.62
   ATOM   968 C   TYR A 127 0   29.328 35.778 21.507 1.00 15.97
   ATOM   969 O   TYR A 127 0   29.626 36.977 21.669 1.00 15.27
   ATOM   970 CB  TYR A 127 0   28.965 34.939 19.176 1.00 14.97
30 ATOM   971 CG  TYR A 127 0   28.057 34.136 18.272 1.00 16.10
   ATOM   972 CD1 TYR A 127 0   27.823 32.782 18.496 1.00 14.96
   ATOM   973 CD2 TYR A 127 0   27.428 34.753 17.177 1.00 16.64
   ATOM   974 CE1 TYR A 127 0   26.995 32.057 17.650 1.00 16.16
   ATOM   975 CE2 TYR A 127 0   26.576 34.039 16.356 1.00 17.32
35 ATOM   976 CZ  TYR A 127 0   26.374 32.692 16.592 1.00 18.16
   ATOM   977 OH  TYR A 127 0   25.540 31.971 15.756 1.00 20.32
   ATOM   978 N   ASP A 128 0   29.892 34.895 22.312 1.00 14.36
   ATOM   979 CA  ASP A 128 0   30.825 35.269 23.365 1.00 16.80
```

ATOM   980 C   ASP A 128 0   32.222 34.863 22.939 1.00 20.11
ATOM   981 O   ASP A 128 0   32.508 33.656 22.777 1.00 21.41
ATOM   982 CB ASP A 128 0   30.398 34.568 24.649 1.00 16.65
ATOM   983 CG ASP A 128 0   31.136 35.055 25.874 1.00 18.36
5 ATOM   984 OD1 ASP A 128 0   32.194 35.708 25.750 1.00 18.72
ATOM   985 OD2 ASP A 128 0   30.710 34.819 27.024 1.00 20.03
ATOM   986 N   ASP A 129 0   33.148 35.798 22.771 1.00 22.30
ATOM   987 CA ASP A 129 0   34.511 35.389 22.377 1.00 24.39
ATOM   988 C   ASP A 129 0   35.282 34.740 23.509 1.00 22.47
10 ATOM   989 O   ASP A 129 0   36.275 34.096 23.209 1.00 23.18
ATOM   990 CB ASP A 129 0   35.298 36.490 21.707 1.00 28.46
ATOM   991 CG ASP A 129 0   35.372 37.764 22.516 1.00 31.10
ATOM   992 OD1 ASP A 129 0   35.254 37.652 23.747 1.00 32.87
ATOM   993 OD2 ASP A 129 0   35.553 38.824 21.891 1.00 34.70
15 ATOM   994 N   ASN A 130 0   34.829 34.684 24.736 1.00 21.92
ATOM   995 CA ASN A 130 0   35.368 34.015 25.874 1.00 23.74
ATOM   996 C   ASN A 130 0   34.382 32.976 26.417 1.00 23.02
ATOM   997 O   ASN A 130 0   34.352 32.684 27.616 1.00 20.14
ATOM   998 CB ASN A 130 0   35.686 35.002 27.028 1.00 26.41
20 ATOM   999 CG ASN A 130 0   36.583 36.127 26.550 1.00 30.99
ATOM   1000 OD1 ASN A 130 0   36.187 37.309 26.486 1.00 33.20
ATOM   1001 ND2 ASN A 130 0   37.818 35.769 26.175 1.00 30.96
ATOM   1002 N   ASP A 131 0   33.533 32.401 25.561 1.00 23.32
ATOM   1003 CA ASP A 131 0   32.476 31.543 26.127 1.00 21.63
25 ATOM   1004 C   ASP A 131 0   33.010 30.514 27.103 1.00 19.56
ATOM   1005 O   ASP A 131 0   33.704 29.569 26.766 1.00 19.71
ATOM   1006 CB ASP A 131 0   31.594 30.877 25.063 1.00 22.97
ATOM   1007 CG ASP A 131 0   30.220 30.487 25.591 1.00 24.48
ATOM   1008 OD1 ASP A 131 0   30.181 29.525 26.397 1.00 26.42
30 ATOM   1009 OD2 ASP A 131 0   29.166 31.051 25.212 1.00 22.66
ATOM   1010 N   PRO A 132 0   32.491 30.548 28.315 1.00 18.77
ATOM   1011 CA PRO A 132 0   32.759 29.611 29.381 1.00 19.41
ATOM   1012 C   PRO A 132 0   32.523 28.141 29.031 1.00 20.89
ATOM   1013 O   PRO A 132 0   33.112 27.250 29.672 1.00 19.99
35 ATOM   1014 CB PRO A 132 0   31.799 29.990 30.531 1.00 18.42
ATOM   1015 CG PRO A 132 0   31.589 31.470 30.263 1.00 16.87
ATOM   1016 CD PRO A 132 0   31.645 31.673 28.778 1.00 16.73
ATOM   1017 N   HIS A 133 0   31.668 27.836 28.063 1.00 19.47

```
   ATOM  1018  CA  HIS A 133  0  31.331 26.465 27.700 1.00 18.79
   ATOM  1019  C   HIS A 133  0  31.887 26.014 26.372 1.00 19.35
   ATOM  1020  O   HIS A 133  0  31.503 24.954 25.826 1.00 18.60
   ATOM  1021  CB  HIS A 133  0  29.789 26.428 27.536 1.00 18.91
 5 ATOM  1022  CG  HIS A 133  0  29.065 26.242 28.815 1.00 18.13
   ATOM  1023  ND1 HIS A 133  0  29.566 25.551 29.877 1.00 19.52
   ATOM  1024  CD2 HIS A 133  0  27.817 26.625 29.183 1.00 19.38
   ATOM  1025  CE1 HIS A 133  0  28.679 25.530 30.855 1.00 20.08
   ATOM  1026  NE2 HIS A 133  0  27.587 26.180 30.457 1.00 19.60
10 ATOM  1027  N   ALA A 134  0  32.840 26.801 25.852 1.00 19.40
   ATOM  1028  CA  ALA A 134  0  33.413 26.465 24.552 1.00 21.88
   ATOM  1029  C   ALA A 134  0  34.080 25.107 24.525 1.00 21.69
   ATOM  1030  O   ALA A 134  0  34.120 24.514 23.439 1.00 21.61
   ATOM  1031  CB  ALA A 134  0  34.418 27.548 24.128 1.00 22.55
15 ATOM  1032  N   ALA A 135  0  34.582 24.527 25.622 1.00 21.96
   ATOM  1033  CA  ALA A 135  0  35.178 23.192 25.483 1.00 23.53
   ATOM  1034  C   ALA A 135  0  34.144 22.096 25.232 1.00 24.47
   ATOM  1035  O   ALA A 135  0  34.488 20.936 24.989 1.00 24.77
   ATOM  1036  CB  ALA A 135  0  35.910 22.820 26.776 1.00 21.92
20 ATOM  1037  N   LEU A 136  0  32.862 22.375 25.457 1.00 24.95
   ATOM  1038  CA  LEU A 136  0  31.800 21.376 25.404 1.00 23.15
   ATOM  1039  C   LEU A 136  0  31.284 21.076 24.016 1.00 20.31
   ATOM  1040  O   LEU A 136  0  30.609 20.054 23.924 1.00 19.62
   ATOM  1041  CB  LEU A 136  0  30.665 21.845 26.318 1.00 24.43
25 ATOM  1042  CG  LEU A 136  0  30.501 21.211 27.686 1.00 27.55
   ATOM  1043  CD1 LEU A 136  0  31.803 20.721 28.285 1.00 25.75
   ATOM  1044  CD2 LEU A 136  0  29.747 22.129 28.644 1.00 26.92
   ATOM  1045  N   TYR A 137  0  31.565 21.888 22.998 1.00 17.05
   ATOM  1046  CA  TYR A 137  0  31.085 21.612 21.662 1.00 16.65
30 ATOM  1047  C   TYR A 137  0  32.076 22.054 20.599 1.00 17.99
   ATOM  1048  O   TYR A 137  0  32.965 22.891 20.794 1.00 18.69
   ATOM  1049  CB  TYR A 137  0  29.724 22.319 21.402 1.00 16.73
   ATOM  1050  CG  TYR A 137  0  29.711 23.760 21.857 1.00 16.24
   ATOM  1051  CD1 TYR A 137  0  29.302 24.108 23.150 1.00 16.00
35 ATOM  1052  CD2 TYR A 137  0  30.159 24.754 21.001 1.00 14.76
   ATOM  1053  CE1 TYR A 137  0  29.355 25.448 23.551 1.00 15.32
   ATOM  1054  CE2 TYR A 137  0  30.165 26.081 21.396 1.00 15.52
   ATOM  1055  CZ  TYR A 137  0  29.759 26.410 22.675 1.00 15.61
```

```
    ATOM  1056 OH  TYR A 137 0  29.782 27.731 23.055 1.00 17.56
    ATOM  1057 N   ASP A 138 0  31.903 21.549 19.393 1.00 19.04
    ATOM  1058 CA  ASP A 138 0  32.733 21.859 18.253 1.00 20.02
    ATOM  1059 C   ASP A 138 0  32.139 22.933 17.364 1.00 21.05
  5 ATOM  1060 O   ASP A 138 0  32.911 23.553 16.631 1.00 21.98
    ATOM  1061 CB  ASP A 138 0  32.836 20.628 17.315 1.00 20.66
    ATOM  1062 CG  ASP A 138 0  33.355 19.455 18.089 1.00 22.79
    ATOM  1063 OD1 ASP A 138 0  32.744 18.404 18.318 1.00 24.88
    ATOM  1064 OD2 ASP A 138 0  34.481 19.675 18.581 1.00 25.34
 10 ATOM  1065 N   GLU A 139 0  30.825 22.957 17.184 1.00 19.73
    ATOM  1066 CA  GLU A 139 0  30.223 23.865 16.213 1.00 21.27
    ATOM  1067 C   GLU A 139 0  29.086 24.668 16.825 1.00 18.97
    ATOM  1068 O   GLU A 139 0  28.306 24.143 17.608 1.00 16.95
    ATOM  1069 CB  GLU A 139 0  29.617 23.164 15.000 1.00 24.71
 15 ATOM  1070 CG  GLU A 139 0  30.509 22.149 14.311 1.00 30.89
    ATOM  1071 CD  GLU A 139 0  31.633 22.868 13.587 1.00 34.42
    ATOM  1072 OE1 GLU A 139 0  31.340 23.869 12.898 1.00 36.87
    ATOM  1073 OE2 GLU A 139 0  32.794 22.457 13.705 1.00 37.60
    ATOM  1074 N   ASP A 140 0  29.057 25.933 16.408 1.00 19.38
 20 ATOM  1075 CA  ASP A 140 0  28.026 26.847 16.912 1.00 17.89
    ATOM  1076 C   ASP A 140 0  27.858 27.901 15.837 1.00 18.87
    ATOM  1077 O   ASP A 140 0  28.705 28.780 15.768 1.00 21.31
    ATOM  1078 CB  ASP A 140 0  28.438 27.399 18.268 1.00 16.26
    ATOM  1079 CG  ASP A 140 0  27.445 28.399 18.858 1.00 16.73
 25 ATOM  1080 OD1 ASP A 140 0  27.854 29.143 19.781 1.00 14.86
    ATOM  1081 OD2 ASP A 140 0  26.287 28.446 18.401 1.00 13.82
    ATOM  1082 N   ASP A 141 0  26.862 27.844 14.972 1.00 17.34
    ATOM  1083 CA  ASP A 141 0  26.750 28.859 13.937 1.00 19.52
    ATOM  1084 C   ASP A 141 0  25.301 29.031 13.520 1.00 19.33
 30 ATOM  1085 O   ASP A 141 0  24.342 28.513 14.115 1.00 17.91
    ATOM  1086 CB  ASP A 141 0  27.681 28.509 12.772 1.00 21.66
    ATOM  1087 CG  ASP A 141 0  27.384 27.151 12.193 1.00 24.87
    ATOM  1088 OD1 ASP A 141 0  28.280 26.521 11.567 1.00 28.90
    ATOM  1089 OD2 ASP A 141 0  26.271 26.604 12.302 1.00 25.89
 35 ATOM  1090 N   GLU A 142 0  25.102 29.688 12.387 1.00 19.21
    ATOM  1091 CA  GLU A 142 0  23.775 29.945 11.880 1.00 20.84
    ATOM  1092 C   GLU A 142 0  23.052 28.636 11.592 1.00 19.95
    ATOM  1093 O   GLU A 142 0  21.844 28.656 11.665 1.00 18.73
```

```
    ATOM  1094 CB  GLU A 142  0  23.771 30.894 10.699 1.00 23.40
    ATOM  1095 CG  GLU A 142  0  24.295 30.301  9.407 1.00 27.22
    ATOM  1096 CD  GLU A 142  0  25.718 30.826  9.221 1.00 32.36
    ATOM  1097 OE1 GLU A 142  0  26.513 30.920 10.206 1.00 31.87
  5 ATOM  1098 OE2 GLU A 142  0  25.968 31.136  8.023 1.00 35.76
    ATOM  1099 N   ASN A 143  0  23.723 27.508 11.378 1.00 20.40
    ATOM  1100 CA  ASN A 143  0  23.105 26.227 11.151 1.00 19.61
    ATOM  1101 C   ASN A 143  0  22.785 25.468 12.421 1.00 18.35
    ATOM  1102 O   ASN A 143  0  22.317 24.337 12.325 1.00 15.65
 10 ATOM  1103 CB  ASN A 143  0  24.024 25.401 10.229 1.00 23.57
    ATOM  1104 CG  ASN A 143  0  24.133 26.067  8.857 1.00 26.63
    ATOM  1105 OD1 ASN A 143  0  25.220 26.376  8.356 1.00 29.89
    ATOM  1106 ND2 ASN A 143  0  23.049 26.342  8.175 1.00 25.46
    ATOM  1107 N   THR A 144  0  23.067 25.974 13.632 1.00 16.76
 15 ATOM  1108 CA  THR A 144  0  22.678 25.257 14.825 1.00 15.40
    ATOM  1109 C   THR A 144  0  21.556 25.976 15.577 1.00 15.58
    ATOM  1110 O   THR A 144  0  21.361 25.776 16.789 1.00 17.88
    ATOM  1111 CB  THR A 144  0  23.848 25.018 15.785 1.00 16.43
    ATOM  1112 OG1 THR A 144  0  24.296 26.270 16.297 1.00 14.82
 20 ATOM  1113 CG2 THR A 144  0  24.935 24.215 15.104 1.00 15.98
    ATOM  1114 N   ILE A 145  0  20.821 26.834 14.898 1.00 13.92
    ATOM  1115 CA  ILE A 145  0  19.697 27.550 15.500 1.00 14.31
    ATOM  1116 C   ILE A 145  0  18.392 26.835 15.139 1.00 13.84
    ATOM  1117 O   ILE A 145  0  18.127 26.478 13.996 1.00 12.32
 25 ATOM  1118 CB  ILE A 145  0  19.641 29.016 15.011 1.00 15.15
    ATOM  1119 CG1 ILE A 145  0  20.881 29.726 15.608 1.00 16.27
    ATOM  1120 CG2 ILE A 145  0  18.346 29.736 15.375 1.00 13.14
    ATOM  1121 CD1 ILE A 145  0  21.256 31.006 14.892 1.00 16.72
    ATOM  1122 N   ILE A 146  0  17.550 26.644 16.141 1.00 13.54
 30 ATOM  1123 CA  ILE A 146  0  16.263 25.983 15.926 1.00 13.70
    ATOM  1124 C   ILE A 146  0  15.167 26.899 16.494 1.00 12.67
    ATOM  1125 O   ILE A 146  0  15.155 27.082 17.714 1.00 10.09
    ATOM  1126 CB  ILE A 146  0  16.183 24.580 16.553 1.00 15.97
    ATOM  1127 CG1 ILE A 146  0  17.280 23.621 16.012 1.00 17.29
 35 ATOM  1128 CG2 ILE A 146  0  14.831 23.937 16.207 1.00 14.52
    ATOM  1129 CD1 ILE A 146  0  17.359 22.340 16.832 1.00 18.45
    ATOM  1130 N   THR A 147  0  14.360 27.507 15.610 1.00 10.81
    ATOM  1131 CA  THR A 147  0  13.240 28.310 16.102 1.00 12.54
```

```
   ATOM 1132 C   THR A 147 0  11.912 27.526 15.988 1.00 13.55
   ATOM 1133 O   THR A 147 0  11.655 26.724 15.076 1.00 12.65
   ATOM 1134 CB  THR A 147 0  13.078 29.642 15.351 1.00 12.37
   ATOM 1135 OG1 THR A 147 0  12.728 29.311 14.005 1.00 10.17
 5 ATOM 1136 CG2 THR A 147 0  14.381 30.479 15.402 1.00 11.93
   ATOM 1137 N   LEU A 148 0  11.062 27.715 16.972 1.00 12.48
   ATOM 1138 CA  LEU A 148 0   9.719 27.171 17.039 1.00 13.90
   ATOM 1139 C   LEU A 148 0   8.719 28.350 16.916 1.00 15.44
   ATOM 1140 O   LEU A 148 0   8.860 29.383 17.579 1.00 15.28
10 ATOM 1141 CB  LEU A 148 0   9.501 26.419 18.340 1.00 12.83
   ATOM 1142 CG  LEU A 148 0  10.502 25.293 18.669 1.00 12.45
   ATOM 1143 CD1 LEU A 148 0  10.154 24.669 19.997 1.00 11.49
   ATOM 1144 CD2 LEU A 148 0  10.552 24.203 17.597 1.00 11.82
   ATOM 1145 N   ALA A 149 0   7.726 28.241 16.053 1.00 14.08
15 ATOM 1146 CA  ALA A 149 0   6.725 29.256 15.825 1.00 15.37
   ATOM 1147 C   ALA A 149 0   5.336 28.658 15.521 1.00 16.78
   ATOM 1148 O   ALA A 149 0   5.198 27.637 14.841 1.00 15.78
   ATOM 1149 CB  ALA A 149 0   7.068 30.127 14.628 1.00 13.22
   ATOM 1150 N   ASP A 150 0   4.337 29.344 16.065 1.00 16.39
20 ATOM 1151 CA  ASP A 150 0   2.941 28.995 15.864 1.00 15.96
   ATOM 1152 C   ASP A 150 0   2.515 29.758 14.624 1.00 16.53
   ATOM 1153 O   ASP A 150 0   2.960 30.905 14.483 1.00 18.17
   ATOM 1154 CB  ASP A 150 0   2.066 29.440 17.027 1.00 16.78
   ATOM 1155 CG  ASP A 150 0   2.345 30.836 17.561 1.00 18.15
25 ATOM 1156 OD1 ASP A 150 0   3.410 31.472 17.347 1.00 16.29
   ATOM 1157 OD2 ASP A 150 0   1.414 31.311 18.264 1.00 17.83
   ATOM 1158 N   TRP A 151 0   1.776 29.157 13.726 1.00 15.62
   ATOM 1159 CA  TRP A 151 0   1.366 29.828 12.499 1.00 14.37
   ATOM 1160 C   TRP A 151 0  -0.140 29.688 12.226 1.00 14.78
30 ATOM 1161 O   TRP A 151 0  -0.679 28.607 12.425 1.00 13.41
   ATOM 1162 CB  TRP A 151 0   2.229 29.239 11.373 1.00 13.56
   ATOM 1163 CG  TRP A 151 0   2.046 30.004 10.097 1.00 13.31
   ATOM 1164 CD1 TRP A 151 0   1.385 29.545  8.991 1.00 13.60
   ATOM 1165 CD2 TRP A 151 0   2.484 31.316  9.806 1.00 15.46
35 ATOM 1166 NE1 TRP A 151 0   1.412 30.497  8.017 1.00 14.49
   ATOM 1167 CE2 TRP A 151 0   2.061 31.605  8.473 1.00 15.53
   ATOM 1168 CE3 TRP A 151 0   3.189 32.294 10.522 1.00 16.28
   ATOM 1169 CZ2 TRP A 151 0   2.306 32.822  7.846 1.00 16.57
```

```
   ATOM  1170 CZ3 TRP A 151 0   3.436 33.505  9.881 1.00 18.22
   ATOM  1171 CH2 TRP A 151 0   3.003 33.766  8.560 1.00 18.00
   ATOM  1172 N   TYR A 152 0  -0.818 30.745 11.812 1.00 15.59
   ATOM  1173 CA  TYR A 152 0  -2.266 30.813 11.614 1.00 17.47
 5 ATOM  1174 C   TYR A 152 0  -2.556 31.086 10.149 1.00 18.79
   ATOM  1175 O   TYR A 152 0  -1.830 31.856  9.521 1.00 19.15
   ATOM  1176 CB  TYR A 152 0  -2.981 31.930 12.434 1.00 16.37
   ATOM  1177 CG  TYR A 152 0  -2.539 31.776 13.887 1.00 16.24
   ATOM  1178 CD1 TYR A 152 0  -1.313 32.303 14.318 1.00 15.22
10 ATOM  1179 CD2 TYR A 152 0  -3.267 30.998 14.767 1.00 15.29
   ATOM  1180 CE1 TYR A 152 0  -0.889 32.135 15.626 1.00 14.67
   ATOM  1181 CE2 TYR A 152 0  -2.831 30.799 16.054 1.00 16.52
   ATOM  1182 CZ  TYR A 152 0  -1.632 31.369 16.474 1.00 16.12
   ATOM  1183 OH  TYR A 152 0  -1.219 31.139 17.771 1.00 16.36
15 ATOM  1184 N   HIS A 153 0  -3.590 30.445  9.599 1.00 20.39
   ATOM  1185 CA  HIS A 153 0  -3.899 30.683  8.181 1.00 21.90
   ATOM  1186 C   HIS A 153 0  -4.642 31.988  7.952 1.00 21.94
   ATOM  1187 O   HIS A 153 0  -4.750 32.386  6.784 1.00 22.32
   ATOM  1188 CB  HIS A 153 0  -4.592 29.483  7.549 1.00 22.29
20 ATOM  1189 CG  HIS A 153 0  -3.651 28.319  7.385 1.00 24.52
   ATOM  1190 ND1 HIS A 153 0  -4.071 27.022  7.258 1.00 24.25
   ATOM  1191 CD2 HIS A 153 0  -2.286 28.274  7.338 1.00 23.32
   ATOM  1192 CE1 HIS A 153 0  -3.034 26.220  7.124 1.00 24.15
   ATOM  1193 NE2 HIS A 153 0  -1.956 26.965  7.178 1.00 24.30
25 ATOM  1194 N   ILE A 154 0  -5.084 32.718  8.972 1.00 21.86
   ATOM  1195 CA  ILE A 154 0  -5.611 34.046  8.686 1.00 24.39
   ATOM  1196 C   ILE A 154 0  -4.904 35.051  9.597 1.00 22.15
   ATOM  1197 O   ILE A 154 0  -4.517 34.732 10.698 1.00 20.15
   ATOM  1198 CB  ILE A 154 0  -7.120 34.281  8.693 1.00 26.43
30 ATOM  1199 CG1 ILE A 154 0  -7.682 34.498 10.099 1.00 27.66
   ATOM  1200 CG2 ILE A 154 0  -7.947 33.251  7.928 1.00 26.60
   ATOM  1201 CD1 ILE A 154 0  -7.312 33.468 11.125 1.00 28.86
   ATOM  1202 N   PRO A 155 0  -4.723 36.255  9.105 1.00 23.79
   ATOM  1203 CA  PRO A 155 0  -4.108 37.361  9.816 1.00 23.66
35 ATOM  1204 C   PRO A 155 0  -4.604 37.435 11.252 1.00 24.59
   ATOM  1205 O   PRO A 155 0  -5.814 37.317 11.539 1.00 24.53
   ATOM  1206 CB  PRO A 155 0  -4.546 38.634  9.077 1.00 24.20
   ATOM  1207 CG  PRO A 155 0  -4.990 38.162  7.733 1.00 23.40
```

```
    ATOM  1208 CD  PRO A 155  0  -5.207 36.672  7.776 1.00 23.41
    ATOM  1209 N   ALA A 156  0  -3.704 37.776 12.178 1.00 24.03
    ATOM  1210 CA  ALA A 156  0  -4.066 37.806 13.588 1.00 25.45
    ATOM  1211 C   ALA A 156  0  -5.262 38.667 13.992 1.00 24.85
  5 ATOM  1212 O   ALA A 156  0  -6.083 38.217 14.798 1.00 22.79
    ATOM  1213 CB  ALA A 156  0  -2.866 38.045 14.492 1.00 24.30
    ATOM  1214 N   PRO A 157  0  -5.393 39.873 13.518 1.00 25.98
    ATOM  1215 CA  PRO A 157  0  -6.521 40.741 13.807 1.00 28.77
    ATOM  1216 C   PRO A 157  0  -7.840 40.092 13.406 1.00 30.78
 10 ATOM  1217 O   PRO A 157  0  -8.798 40.416 14.105 1.00 34.62
    ATOM  1218 CB  PRO A 157  0  -6.324 42.071 13.068 1.00 26.56
    ATOM  1219 CG  PRO A 157  0  -4.859 42.013 12.762 1.00 25.98
    ATOM  1220 CD  PRO A 157  0  -4.480 40.547 12.585 1.00 25.96
    ATOM  1221 N   SER A 158  0  -7.950 39.207 12.430 1.00 30.95
 15 ATOM  1222 CA  SER A 158  0  -9.174 38.549 12.047 1.00 31.32
    ATOM  1223 C   SER A 158  0  -9.450 37.288 12.851 1.00 33.61
    ATOM  1224 O   SER A 158  0 -10.472 36.633 12.575 1.00 34.71
    ATOM  1225 CB  SER A 158  0  -9.176 38.118 10.577 1.00 30.14
    ATOM  1226 OG  SER A 158  0  -8.942 39.187  9.665 1.00 31.20
 20 ATOM  1227 N   ILE A 159  0  -8.588 36.875 13.773 1.00 34.23
    ATOM  1228 CA  ILE A 159  0  -8.918 35.642 14.491 1.00 36.40
    ATOM  1229 C   ILE A 159  0 -10.189 35.896 15.309 1.00 39.20
    ATOM  1230 O   ILE A 159  0 -10.294 36.875 16.046 1.00 39.00
    ATOM  1231 CB  ILE A 159  0  -7.769 35.121 15.360 1.00 35.56
 25 ATOM  1232 CG1 ILE A 159  0  -6.713 34.408 14.485 1.00 35.58
    ATOM  1233 CG2 ILE A 159  0  -8.262 34.184 16.452 1.00 34.97
    ATOM  1234 CD1 ILE A 159  0  -5.388 34.268 15.212 1.00 34.91
    ATOM  1235 N   GLN A 160  0 -11.137 34.969 15.196 1.00 41.53
    ATOM  1236 CA  GLN A 160  0 -12.398 35.056 15.946 1.00 42.57
 30 ATOM  1237 C   GLN A 160  0 -12.466 33.914 16.949 1.00 40.51
    ATOM  1238 O   GLN A 160  0 -12.308 32.741 16.585 1.00 41.96
    ATOM  1239 CB  GLN A 160  0 -13.542 35.062 14.937 1.00 45.52
    ATOM  1240 CG  GLN A 160  0 -14.814 34.319 15.267 1.00 48.48
    ATOM  1241 CD  GLN A 160  0 -15.570 33.799 14.055 1.00 50.12
 35 ATOM  1242 OE1 GLN A 160  0 -16.204 32.737 14.118 1.00 50.77
    ATOM  1243 NE2 GLN A 160  0 -15.504 34.520 12.940 1.00 51.22
    ATOM  1244 N   GLY A 161  0 -12.667 34.191 18.225 1.00 37.10
    ATOM  1245 CA  GLY A 161  0 -12.722 33.112 19.208 1.00 34.91
```

ATOM 1246 C GLY A 161 0 -11.305 32.826 19.696 1.00 34.13
ATOM 1247 O GLY A 161 0 -10.412 33.648 19.451 1.00 32.40
ATOM 1248 N ALA A 162 0 -11.158 31.738 20.433 1.00 33.01
ATOM 1249 CA ALA A 162 0 -9.864 31.355 20.988 1.00 32.39
5 ATOM 1250 C ALA A 162 0 -8.927 30.902 19.880 1.00 31.53
ATOM 1251 O ALA A 162 0 -9.285 30.132 19.013 1.00 30.73
ATOM 1252 CB ALA A 162 0 -10.058 30.263 22.010 1.00 34.12
ATOM 1253 N ALA A 163 0 -7.731 31.475 19.851 1.00 32.06
ATOM 1254 CA ALA A 163 0 -6.740 31.202 18.814 1.00 30.85
10 ATOM 1255 C ALA A 163 0 -6.219 29.774 18.897 1.00 29.40
ATOM 1256 O ALA A 163 0 -5.967 29.223 19.965 1.00 30.49
ATOM 1257 CB ALA A 163 0 -5.607 32.217 18.911 1.00 30.29
ATOM 1258 N GLN A 164 0 -6.101 29.130 17.754 1.00 28.69
ATOM 1259 CA GLN A 164 0 -5.616 27.769 17.612 1.00 28.24
15 ATOM 1260 C GLN A 164 0 -4.720 27.744 16.370 1.00 25.02
ATOM 1261 O GLN A 164 0 -5.157 28.046 15.260 1.00 23.64
ATOM 1262 CB GLN A 164 0 -6.732 26.756 17.361 1.00 31.99
ATOM 1263 CG GLN A 164 0 -7.885 26.640 18.319 1.00 36.24
ATOM 1264 CD GLN A 164 0 -7.535 25.809 19.540 1.00 40.95
20 ATOM 1265 OE1 GLN A 164 0 -7.863 26.166 20.684 1.00 43.34
ATOM 1266 NE2 GLN A 164 0 -6.864 24.672 19.328 1.00 41.86
ATOM 1267 N PRO A 165 0 -3.446 27.406 16.549 1.00 22.68
ATOM 1268 CA PRO A 165 0 -2.501 27.360 15.463 1.00 20.43
ATOM 1269 C PRO A 165 0 -2.856 26.294 14.429 1.00 18.89
25 ATOM 1270 O PRO A 165 0 -3.286 25.176 14.715 1.00 18.00
ATOM 1271 CB PRO A 165 0 -1.126 27.075 16.088 1.00 20.83
ATOM 1272 CG PRO A 165 0 -1.476 26.651 17.479 1.00 22.05
ATOM 1273 CD PRO A 165 0 -2.873 27.081 17.851 1.00 21.57
ATOM 1274 N ASP A 166 0 -2.667 26.608 13.169 1.00 17.50
30 ATOM 1275 CA ASP A 166 0 -2.829 25.677 12.059 1.00 19.82
ATOM 1276 C ASP A 166 0 -1.591 24.788 11.930 1.00 19.47
ATOM 1277 O ASP A 166 0 -1.692 23.649 11.506 1.00 19.38
ATOM 1278 CB ASP A 166 0 -3.005 26.413 10.727 1.00 19.75
ATOM 1279 CG ASP A 166 0 -4.347 27.162 10.728 1.00 21.69
35 ATOM 1280 OD1 ASP A 166 0 -5.376 26.480 10.593 1.00 22.24
ATOM 1281 OD2 ASP A 166 0 -4.384 28.392 10.885 1.00 22.13
ATOM 1282 N ALA A 167 0 -0.435 25.386 12.231 1.00 18.54
ATOM 1283 CA ALA A 167 0 0.806 24.614 12.142 1.00 18.74

```
   ATOM 1284 C   ALA A 167 0   1.867 25.056 13.148 1.00 17.69
   ATOM 1285 O   ALA A 167 0   1.874 26.147 13.715 1.00 15.83
   ATOM 1286 CB  ALA A 167 0   1.387 24.767 10.735 1.00 17.32
   ATOM 1287 N   THR A 168 0   2.826 24.166 13.335 1.00 18.40
 5 ATOM 1288 CA  THR A 168 0   4.087 24.402 14.027 1.00 14.85
   ATOM 1289 C   THR A 168 0   5.180 24.553 12.955 1.00 15.24
   ATOM 1290 O   THR A 168 0   5.402 23.737 12.071 1.00 12.99
   ATOM 1291 CB  THR A 168 0   4.530 23.235 14.900 1.00 14.31
   ATOM 1292 OG1 THR A 168 0   3.558 23.068 15.920 1.00 12.30
10 ATOM 1293 CG2 THR A 168 0   5.921 23.516 15.524 1.00 13.60
   ATOM 1294 N   LEU A 169 0   5.867 25.686 12.973 1.00 16.69
   ATOM 1295 CA  LEU A 169 0   6.976 26.002 12.071 1.00 14.74
   ATOM 1296 C   LEU A 169 0   8.285 25.747 12.833 1.00 14.34
   ATOM 1297 O   LEU A 169 0   8.497 26.259 13.942 1.00 12.34
15 ATOM 1298 CB  LEU A 169 0   6.890 27.471 11.652 1.00 14.90
   ATOM 1299 CG  LEU A 169 0   6.071 27.845 10.428 1.00 17.83
   ATOM 1300 CD1 LEU A 169 0   4.978 26.825 10.133 1.00 15.89
   ATOM 1301 CD2 LEU A 169 0   5.500 29.254 10.443 1.00 16.43
   ATOM 1302 N   ILE A 170 0   9.141 24.923 12.255 1.00 14.06
20 ATOM 1303 CA  ILE A 170 0  10.472 24.659 12.819 1.00 14.01
   ATOM 1304 C   ILE A 170 0  11.397 25.312 11.784 1.00 15.19
   ATOM 1305 O   ILE A 170 0  11.307 25.009 10.585 1.00 14.73
   ATOM 1306 CB  ILE A 170 0  10.807 23.179 13.025 1.00 14.75
   ATOM 1307 CG1 ILE A 170 0   9.849 22.605 14.069 1.00 13.74
25 ATOM 1308 CG2 ILE A 170 0  12.268 22.983 13.468 1.00 13.47
   ATOM 1309 CD1 ILE A 170 0   9.915 21.134 14.385 1.00 15.26
   ATOM 1310 N   ASN A 171 0  12.166 26.317 12.208 1.00 13.13
   ATOM 1311 CA  ASN A 171 0  12.992 27.042 11.250 1.00 13.74
   ATOM 1312 C   ASN A 171 0  12.163 27.517 10.083 1.00 13.71
30 ATOM 1313 O   ASN A 171 0  12.562 27.381  8.921 1.00 13.20
   ATOM 1314 CB  ASN A 171 0  14.220 26.209 10.793 1.00 14.42
   ATOM 1315 CG  ASN A 171 0  15.236 26.157 11.940 1.00 16.29
   ATOM 1316 OD1 ASN A 171 0  15.123 26.983 12.875 1.00 16.78
   ATOM 1317 ND2 ASN A 171 0  16.203 25.259 11.964 1.00 14.32
35 ATOM 1318 N   GLY A 172 0  10.967 28.074 10.337 1.00 14.17
   ATOM 1319 CA  GLY A 172 0  10.157 28.619  9.270 1.00 11.74
   ATOM 1320 C   GLY A 172 0   9.387 27.636  8.433 1.00 14.40
   ATOM 1321 O   GLY A 172 0   8.783 28.064  7.441 1.00 15.60
```

```
   ATOM  1322 N   LYS A 173 0   9.430 26.319  8.669 1.00 13.84
   ATOM  1323 CA  LYS A 173 0   8.777 25.363  7.794 1.00 13.67
   ATOM  1324 C   LYS A 173 0   8.038 24.303  8.589 1.00 13.59
   ATOM  1325 O   LYS A 173 0   8.445 24.027  9.723 1.00 11.70
 5 ATOM  1326 CB  LYS A 173 0   9.775 24.645  6.875 1.00 17.03
   ATOM  1327 CG  LYS A 173 0  10.704 25.577  6.118 1.00 17.63
   ATOM  1328 CD  LYS A 173 0  11.508 24.796  5.094 1.00 20.84
   ATOM  1329 CE  LYS A 173 0  12.213 25.821  4.198 1.00 22.63
   ATOM  1330 NZ  LYS A 173 0  13.304 25.087  3.499 1.00 28.08
10 ATOM  1331 N   GLY A 174 0   6.922 23.821  8.014 1.00 12.28
   ATOM  1332 CA  GLY A 174 0   6.178 22.768  8.753 1.00 11.45
   ATOM  1333 C   GLY A 174 0   4.958 22.409  7.896 1.00 13.55
   ATOM  1334 O   GLY A 174 0   4.823 22.877  6.760 1.00 13.37
   ATOM  1335 N   ARG A 175 0   4.042 21.619  8.432 1.00 14.54
15 ATOM  1336 CA  ARG A 175 0   2.859 21.201  7.687 1.00 16.62
   ATOM  1337 C   ARG A 175 0   1.598 21.336  8.541 1.00 17.67
   ATOM  1338 O   ARG A 175 0   1.727 21.264  9.769 1.00 18.41
   ATOM  1339 CB  ARG A 175 0   2.985 19.718  7.292 1.00 16.05
   ATOM  1340 CG  ARG A 175 0   3.894 19.472  6.116 1.00 16.55
20 ATOM  1341 CD  ARG A 175 0   4.358 18.009  6.108 1.00 17.70
   ATOM  1342 NE  ARG A 175 0   5.421 17.861  5.097 1.00 17.74
   ATOM  1343 CZ  ARG A 175 0   5.971 16.667  4.792 1.00 17.63
   ATOM  1344 NH1 ARG A 175 0   6.918 16.665  3.866 1.00 17.25
   ATOM  1345 NH2 ARG A 175 0   5.594 15.538  5.375 1.00 14.80
25 ATOM  1346 N   TYR A 176 0   0.429 21.438  7.908 1.00 18.08
   ATOM  1347 CA  TYR A 176 0  -0.800 21.481  8.746 1.00 18.67
   ATOM  1348 C   TYR A 176 0  -1.613 20.200  8.509 1.00 18.24
   ATOM  1349 O   TYR A 176 0  -1.417 19.534  7.483 1.00 17.67
   ATOM  1350 CB  TYR A 176 0  -1.635 22.709  8.462 1.00 17.21
30 ATOM  1351 CG  TYR A 176 0  -2.102 22.931  7.053 1.00 16.36
   ATOM  1352 CD1 TYR A 176 0  -1.246 23.433  6.089 1.00 14.84
   ATOM  1353 CD2 TYR A 176 0  -3.441 22.676  6.677 1.00 17.26
   ATOM  1354 CE1 TYR A 176 0  -1.640 23.686  4.796 1.00 16.01
   ATOM  1355 CE2 TYR A 176 0  -3.862 22.908  5.361 1.00 16.65
35 ATOM  1356 CZ  TYR A 176 0  -2.967 23.407  4.432 1.00 17.65
   ATOM  1357 OH  TYR A 176 0  -3.347 23.678  3.131 1.00 17.81
   ATOM  1358 N   VAL A 177 0  -2.427 19.815  9.464 1.00 18.46
   ATOM  1359 CA  VAL A 177 0  -3.200 18.571  9.303 1.00 21.18
```

```
ATOM   1360  C   VAL A 177  0   -4.090  18.639   8.073  1.00 21.50
ATOM   1361  O   VAL A 177  0   -4.788  19.620   7.858  1.00 21.85
ATOM   1362  CB  VAL A 177  0   -4.072  18.306  10.532  1.00 22.29
ATOM   1363  CG1 VAL A 177  0   -4.802  16.974  10.370  1.00 21.70
ATOM   1364  CG2 VAL A 177  0   -3.205  18.289  11.784  1.00 22.43
ATOM   1365  N   GLY A 178  0   -3.989  17.707   7.142  1.00 21.84
ATOM   1366  CA  GLY A 178  0   -4.761  17.742   5.918  1.00 20.35
ATOM   1367  C   GLY A 178  0   -4.047  18.602   4.900  1.00 22.84
ATOM   1368  O   GLY A 178  0   -4.576  18.673   3.774  1.00 23.86
ATOM   1369  N   GLY A 179  0   -2.887  19.220   5.210  1.00 21.49
ATOM   1370  CA  GLY A 179  0   -2.291  20.060   4.149  1.00 19.94
ATOM   1371  C   GLY A 179  0   -1.389  19.250   3.242  1.00 18.86
ATOM   1372  O   GLY A 179  0   -1.192  18.052   3.399  1.00 19.35
ATOM   1373  N   PRO A 180  0   -0.800  19.905   2.268  1.00 19.42
ATOM   1374  CA  PRO A 180  0    0.150  19.328   1.335  1.00 19.92
ATOM   1375  C   PRO A 180  0    1.430  18.922   2.041  1.00 20.56
ATOM   1376  O   PRO A 180  0    1.731  19.399   3.145  1.00 20.66
ATOM   1377  CB  PRO A 180  0    0.503  20.399   0.298  1.00 19.52
ATOM   1378  CG  PRO A 180  0   -0.144  21.639   0.829  1.00 19.70
ATOM   1379  CD  PRO A 180  0   -0.930  21.356   2.081  1.00 19.79
ATOM   1380  N   ALA A 181  0    2.213  18.059   1.403  1.00 21.19
ATOM   1381  CA  ALA A 181  0    3.489  17.644   2.007  1.00 23.04
ATOM   1382  C   ALA A 181  0    4.548  18.723   1.772  1.00 21.24
ATOM   1383  O   ALA A 181  0    5.465  18.522   0.986  1.00 23.93
ATOM   1384  CB  ALA A 181  0    3.928  16.305   1.435  1.00 21.73
ATOM   1385  N   ALA A 182  0    4.398  19.905   2.315  1.00 19.30
ATOM   1386  CA  ALA A 182  0    5.357  20.987   2.183  1.00 18.39
ATOM   1387  C   ALA A 182  0    6.706  20.549   2.791  1.00 17.36
ATOM   1388  O   ALA A 182  0    6.858  19.712   3.701  1.00 16.16
ATOM   1389  CB  ALA A 182  0    4.826  22.209   2.932  1.00 17.68
ATOM   1390  N   GLU A 183  0    7.739  21.103   2.210  1.00 18.23
ATOM   1391  CA  GLU A 183  0    9.134  20.882   2.599  1.00 20.90
ATOM   1392  C   GLU A 183  0    9.381  21.078   4.093  1.00 18.87
ATOM   1393  O   GLU A 183  0    8.976  22.073   4.699  1.00 17.80
ATOM   1394  CB  GLU A 183  0    9.990  21.875   1.820  1.00 25.16
ATOM   1395  CG  GLU A 183  0   11.508  21.760   1.962  1.00 31.31
ATOM   1396  CD  GLU A 183  0   12.075  22.803   0.998  1.00 34.38
ATOM   1397  OE1 GLU A 183  0   11.901  22.609  -0.229  1.00 36.88
```

ATOM   1398 OE2 GLU A 183 0   12.619 23.809 1.484 1.00 36.18
ATOM   1399 N   LEU A 184 0   10.010 20.093 4.691 1.00 17.33
ATOM   1400 CA LEU A 184 0   10.388 20.155 6.098 1.00 18.77
ATOM   1401 C   LEU A 184 0   11.780 20.743 6.255 1.00 19.44
5 ATOM 1402 O   LEU A 184 0   12.582 20.687 5.314 1.00 20.95
ATOM   1403 CB LEU A 184 0   10.331 18.735 6.673 1.00 18.11
ATOM   1404 CG LEU A 184 0   8.915 18.125 6.577 1.00 19.10
ATOM   1405 CD1 LEU A 184 0   8.887 16.734 7.178 1.00 18.87
ATOM   1406 CD2 LEU A 184 0   7.868 19.026 7.229 1.00 18.69
10 ATOM 1407 N   SER A 185 0   12.054 21.342 7.398 1.00 18.46
ATOM   1408 CA SER A 185 0   13.366 21.883 7.699 1.00 17.73
ATOM   1409 C   SER A 185 0   14.298 20.699 8.018 1.00 16.95
ATOM   1410 O   SER A 185 0   13.883 19.710 8.629 1.00 15.84
ATOM   1411 CB SER A 185 0   13.303 22.786 8.934 1.00 17.34
15 ATOM 1412 OG SER A 185 0   12.846 24.073 8.560 1.00 18.09
ATOM   1413 N   ILE A 186 0   15.533 20.845 7.587 1.00 16.43
ATOM   1414 CA ILE A 186 0   16.595 19.858 7.821 1.00 16.85
ATOM   1415 C   ILE A 186 0   17.725 20.491 8.626 1.00 15.86
ATOM   1416 O   ILE A 186 0   18.178 21.605 8.387 1.00 11.67
20 ATOM 1417 CB ILE A 186 0   17.193 19.390 6.471 1.00 18.77
ATOM   1418 CG1 ILE A 186 0   16.048 18.895 5.557 1.00 19.78
ATOM   1419 CG2 ILE A 186 0   18.167 18.241 6.697 1.00 18.53
ATOM   1420 CD1 ILE A 186 0   16.464 18.731 4.110 1.00 22.35
ATOM   1421 N   VAL A 187 0   18.114 19.840 9.703 1.00 16.18
25 ATOM 1422 CA VAL A 187 0   19.243 20.287 10.505 1.00 16.63
ATOM   1423 C   VAL A 187 0   20.362 19.239 10.231 1.00 17.36
ATOM   1424 O   VAL A 187 0   20.158 18.046 10.505 1.00 15.19
ATOM   1425 CB VAL A 187 0   18.928 20.323 11.984 1.00 16.68
ATOM   1426 CG1 VAL A 187 0   20.198 20.622 12.796 1.00 16.82
30 ATOM 1427 CG2 VAL A 187 0   17.874 21.375 12.275 1.00 17.07
ATOM   1428 N   ASN A 188 0   21.449 19.695 9.634 1.00 16.45
ATOM   1429 CA ASN A 188 0   22.528 18.766 9.272 1.00 19.84
ATOM   1430 C   ASN A 188 0   23.598 18.597 10.349 1.00 19.41
ATOM   1431 O   ASN A 188 0   24.051 19.618 10.862 1.00 21.31
35 ATOM 1432 CB ASN A 188 0   23.209 19.246 7.976 1.00 18.78
ATOM   1433 CG ASN A 188 0   22.249 19.186 6.797 1.00 20.77
ATOM   1434 OD1 ASN A 188 0   21.734 20.201 6.305 1.00 21.70
ATOM   1435 ND2 ASN A 188 0   21.995 17.985 6.286 1.00 20.52

```
   ATOM  1436 N   VAL A 189  0  24.024 17.389 10.681 1.00 17.35
   ATOM  1437 CA  VAL A 189  0  25.098 17.164 11.617 1.00 17.93
   ATOM  1438 C   VAL A 189  0  26.091 16.135 11.046 1.00 19.82
   ATOM  1439 O   VAL A 189  0  25.773 15.392 10.109 1.00 18.90
 5 ATOM  1440 CB  VAL A 189  0  24.660 16.684 13.009 1.00 18.43
   ATOM  1441 CG1 VAL A 189  0  23.931 17.796 13.766 1.00 18.89
   ATOM  1442 CG2 VAL A 189  0  23.760 15.449 12.965 1.00 15.94
   ATOM  1443 N   GLU A 190  0  27.242 15.993 11.688 1.00 21.48
   ATOM  1444 CA  GLU A 190  0  28.220 14.972 11.274 1.00 24.63
10 ATOM  1445 C   GLU A 190  0  28.514 14.065 12.469 1.00 23.06
   ATOM  1446 O   GLU A 190  0  28.797 14.650 13.522 1.00 21.04
   ATOM  1447 CB  GLU A 190  0  29.569 15.551 10.860 1.00 26.79
   ATOM  1448 CG  GLU A 190  0  29.571 16.355  9.567 1.00 32.24
   ATOM  1449 CD  GLU A 190  0  30.951 16.990  9.351 1.00 34.67
15 ATOM  1450 OE1 GLU A 190  0  31.927 16.199  9.305 1.00 35.41
   ATOM  1451 OE2 GLU A 190  0  30.999 18.236  9.264 1.00 35.78
   ATOM  1452 N   GLN A 191  0  28.490 12.752 12.256 1.00 21.94
   ATOM  1453 CA  GLN A 191  0  28.768 11.824 13.357 1.00 21.92
   ATOM  1454 C   GLN A 191  0  30.121 12.151 13.984 1.00 22.68
20 ATOM  1455 O   GLN A 191  0  31.052 12.516 13.251 1.00 23.08
   ATOM  1456 CB  GLN A 191  0  28.797 10.400 12.820 1.00 22.01
   ATOM  1457 CG  GLN A 191  0  28.795  9.347 13.917 1.00 23.87
   ATOM  1458 CD  GLN A 191  0  28.846  7.966 13.259 1.00 26.64
   ATOM  1459 OE1 GLN A 191  0  29.745  7.761 12.427 1.00 28.86
25 ATOM  1460 NE2 GLN A 191  0  27.909  7.080 13.563 1.00 26.40
   ATOM  1461 N   GLY A 192  0  30.224 12.119 15.290 1.00 21.84
   ATOM  1462 CA  GLY A 192  0  31.418 12.469 15.996 1.00 22.91
   ATOM  1463 C   GLY A 192  0  31.564 13.910 16.446 1.00 23.87
   ATOM  1464 O   GLY A 192  0  32.394 14.174 17.322 1.00 25.80
30 ATOM  1465 N   LYS A 193  0  30.839 14.867 15.922 1.00 23.54
   ATOM  1466 CA  LYS A 193  0  30.899 16.259 16.362 1.00 22.84
   ATOM  1467 C   LYS A 193  0  29.840 16.584 17.404 1.00 21.67
   ATOM  1468 O   LYS A 193  0  28.826 15.882 17.538 1.00 20.99
   ATOM  1469 CB  LYS A 193  0  30.682 17.155 15.143 1.00 24.53
35 ATOM  1470 CG  LYS A 193  0  31.900 17.149 14.217 1.00 27.82
   ATOM  1471 CD  LYS A 193  0  31.739 18.261 13.199 1.00 30.02
   ATOM  1472 CE  LYS A 193  0  33.060 19.001 12.990 1.00 31.93
   ATOM  1473 NZ  LYS A 193  0  33.392 18.906 11.540 1.00 33.14
```

```
    ATOM  1474 N   LYS A 194 0  30.067 17.626 18.169 1.00 19.25
    ATOM  1475 CA  LYS A 194 0  29.168 18.115 19.187 1.00 19.49
    ATOM  1476 C   LYS A 194 0  28.722 19.523 18.780 1.00 19.40
    ATOM  1477 O   LYS A 194 0  29.512 20.285 18.235 1.00 19.29
  5 ATOM  1478 CB  LYS A 194 0  29.771 18.115 20.576 1.00 21.88
    ATOM  1479 CG  LYS A 194 0  30.338 16.748 20.999 1.00 25.59
    ATOM  1480 CD  LYS A 194 0  31.054 16.902 22.331 1.00 29.48
    ATOM  1481 CE  LYS A 194 0  31.455 15.582 22.970 1.00 33.58
    ATOM  1482 NZ  LYS A 194 0  30.363 15.049 23.868 1.00 35.93
 10 ATOM  1483 N   TYR A 195 0  27.418 19.818 18.910 1.00 16.92
    ATOM  1484 CA  TYR A 195 0  26.858 21.068 18.431 1.00 15.60
    ATOM  1485 C   TYR A 195 0  26.143 21.838 19.530 1.00 14.20
    ATOM  1486 O   TYR A 195 0  25.394 21.232 20.295 1.00 13.75
    ATOM  1487 CB  TYR A 195 0  25.814 20.880 17.300 1.00 16.13
 15 ATOM  1488 CG  TYR A 195 0  26.424 20.225 16.066 1.00 15.41
    ATOM  1489 CD1 TYR A 195 0  26.663 18.851 16.091 1.00 15.91
    ATOM  1490 CD2 TYR A 195 0  26.786 20.942 14.945 1.00 14.73
    ATOM  1491 CE1 TYR A 195 0  27.244 18.204 15.010 1.00 16.55
    ATOM  1492 CE2 TYR A 195 0  27.331 20.312 13.839 1.00 15.60
 20 ATOM  1493 CZ  TYR A 195 0  27.570 18.947 13.888 1.00 16.18
    ATOM  1494 OH  TYR A 195 0  28.144 18.287 12.831 1.00 15.64
    ATOM  1495 N   ARG A 196 0  26.366 23.136 19.561 1.00 12.74
    ATOM  1496 CA  ARG A 196 0  25.619 23.980 20.482 1.00 13.63
    ATOM  1497 C   ARG A 196 0  24.343 24.369 19.711 1.00 13.86
 25 ATOM  1498 O   ARG A 196 0  24.343 25.218 18.802 1.00 13.81
    ATOM  1499 CB  ARG A 196 0  26.379 25.187 20.991 1.00 13.96
    ATOM  1500 CG  ARG A 196 0  25.520 26.162 21.796 1.00 14.22
    ATOM  1501 CD  ARG A 196 0  26.337 27.238 22.438 1.00 15.27
    ATOM  1502 NE  ARG A 196 0  25.649 28.138 23.319 1.00 17.38
 30 ATOM  1503 CZ  ARG A 196 0  26.203 29.034 24.140 1.00 18.86
    ATOM  1504 NH1 ARG A 196 0  27.540 29.141 24.217 1.00 16.30
    ATOM  1505 NH2 ARG A 196 0  25.377 29.788 24.869 1.00 16.73
    ATOM  1506 N   MET A 197 0  23.266 23.624 20.002 1.00 13.86
    ATOM  1507 CA  MET A 197 0  21.980 23.932 19.340 1.00 12.98
 35 ATOM  1508 C   MET A 197 0  21.293 25.055 20.127 1.00 12.50
    ATOM  1509 O   MET A 197 0  21.285 24.997 21.359 1.00 13.93
    ATOM  1510 CB  MET A 197 0  21.118 22.693 19.266 1.00 12.50
    ATOM  1511 CG  MET A 197 0  21.762 21.567 18.447 1.00 13.94
```

```
   ATOM  1512 SD  MET A 197 0  21.860 22.033 16.735 1.00 16.62
   ATOM  1513 CE  MET A 197 0  22.157 20.467 15.927 1.00 16.37
   ATOM  1514 N   ARG A 198 0  20.768 26.064 19.450 1.00 11.00
   ATOM  1515 CA  ARG A 198 0  20.131 27.191 20.137 1.00 11.83
5  ATOM  1516 C   ARG A 198 0  18.624 27.130 19.868 1.00 12.36
   ATOM  1517 O   ARG A 198 0  18.145 27.304 18.731 1.00 10.03
   ATOM  1518 CB  ARG A 198 0  20.804 28.460 19.629 1.00 13.98
   ATOM  1519 CG  ARG A 198 0  22.282 28.567 20.065 1.00 16.25
   ATOM  1520 CD  ARG A 198 0  22.932 29.863 19.626 1.00 16.68
10 ATOM  1521 NE  ARG A 198 0  24.350 29.957 20.042 1.00 16.91
   ATOM  1522 CZ  ARG A 198 0  24.812 30.691 21.055 1.00 15.76
   ATOM  1523 NH1 ARG A 198 0  24.031 31.456 21.820 1.00 13.44
   ATOM  1524 NH2 ARG A 198 0  26.123 30.721 21.316 1.00 15.41
   ATOM  1525 N   LEU A 199 0  17.871 26.807 20.908 1.00 10.44
15 ATOM  1526 CA  LEU A 199 0  16.426 26.568 20.708 1.00 10.69
   ATOM  1527 C   LEU A 199 0  15.598 27.772 21.169 1.00 10.07
   ATOM  1528 O   LEU A 199 0  15.682 28.216 22.317 1.00 10.07
   ATOM  1529 CB  LEU A 199 0  16.003 25.317 21.491 1.00  8.67
   ATOM  1530 CG  LEU A 199 0  14.499 24.942 21.391 1.00 10.33
20 ATOM  1531 CD1 LEU A 199 0  14.193 24.333 20.023 1.00  8.13
   ATOM  1532 CD2 LEU A 199 0  14.170 23.907 22.485 1.00  9.10
   ATOM  1533 N   ILE A 200 0  14.857 28.370 20.242 1.00 10.46
   ATOM  1534 CA  ILE A 200 0  14.104 29.572 20.585 1.00 11.72
   ATOM  1535 C   ILE A 200 0  12.627 29.428 20.310 1.00 13.84
25 ATOM  1536 O   ILE A 200 0  12.254 29.059 19.192 1.00 13.22
   ATOM  1537 CB  ILE A 200 0  14.628 30.755 19.735 1.00 12.89
   ATOM  1538 CG1 ILE A 200 0  16.165 30.899 19.824 1.00 12.38
   ATOM  1539 CG2 ILE A 200 0  13.998 32.091 20.065 1.00 13.13
   ATOM  1540 CD1 ILE A 200 0  16.811 31.634 18.671 1.00 12.54
30 ATOM  1541 N   SER A 201 0  11.829 29.825 21.312 1.00 14.64
   ATOM  1542 CA  SER A 201 0  10.379 29.849 21.023 1.00 13.89
   ATOM  1543 C   SER A 201 0  10.018 31.280 20.608 1.00 11.10
   ATOM  1544 O   SER A 201 0  10.250 32.261 21.320 1.00  8.85
   ATOM  1545 CB  SER A 201 0   9.539 29.367 22.202 1.00 13.01
35 ATOM  1546 OG  SER A 201 0   8.313 30.047 22.207 1.00 12.19
   ATOM  1547 N   LEU A 202 0   9.428 31.376 19.438 1.00  9.64
   ATOM  1548 CA  LEU A 202 0   8.959 32.637 18.881 1.00  9.06
   ATOM  1549 C   LEU A 202 0   7.415 32.740 19.046 1.00 10.40
```

```
    ATOM 1550 O   LEU A 202 0   6.802 33.528 18.351 1.00 9.36
    ATOM 1551 CB  LEU A 202 0   9.239 32.618 17.379 1.00 9.09
    ATOM 1552 CG  LEU A 202 0  10.691 32.451 16.888 1.00 10.90
    ATOM 1553 CD1 LEU A 202 0  10.637 32.470 15.367 1.00 10.05
  5 ATOM 1554 CD2 LEU A 202 0  11.617 33.559 17.414 1.00 8.56
    ATOM 1555 N   SER A 203 0   6.821 31.942 19.892 1.00 9.59
    ATOM 1556 CA  SER A 203 0   5.414 31.756 20.017 1.00 15.31
    ATOM 1557 C   SER A 203 0   4.624 32.960 20.544 1.00 16.67
    ATOM 1558 O   SER A 203 0   4.964 33.676 21.483 1.00 16.42
 10 ATOM 1559 CB  SER A 203 0   5.130 30.505 20.867 1.00 15.21
    ATOM 1560 OG  SER A 203 0   3.742 30.240 21.004 1.00 17.14
    ATOM 1561 N   CYS A 204 0   3.428 33.051 19.984 1.00 17.18
    ATOM 1562 CA  CYS A 204 0   2.442 34.018 20.470 1.00 18.43
    ATOM 1563 C   CYS A 204 0   1.599 33.316 21.522 1.00 17.02
 15 ATOM 1564 O   CYS A 204 0   0.867 34.039 22.200 1.00 17.27
    ATOM 1565 CB  CYS A 204 0   1.524 34.508 19.334 1.00 18.60
    ATOM 1566 SG  CYS A 204 0   2.135 36.038 18.612 1.00 20.23
    ATOM 1567 N   ASP A 205 0   1.687 31.989 21.665 1.00 16.38
    ATOM 1568 CA  ASP A 205 0   0.776 31.392 22.683 1.00 12.26
 20 ATOM 1569 C   ASP A 205 0   1.123 30.002 23.087 1.00 11.34
    ATOM 1570 O   ASP A 205 0   1.432 29.687 24.255 1.00 11.40
    ATOM 1571 CB  ASP A 205 0  -0.622 31.516 22.076 1.00 14.87
    ATOM 1572 CG  ASP A 205 0  -1.729 30.881 22.892 1.00 16.61
    ATOM 1573 OD1 ASP A 205 0  -2.884 30.999 22.433 1.00 18.48
 25 ATOM 1574 OD2 ASP A 205 0  -1.534 30.263 23.966 1.00 17.48
    ATOM 1575 N   PRO A 206 0   1.036 29.030 22.205 1.00 11.79
    ATOM 1576 CA  PRO A 206 0   1.313 27.639 22.542 1.00 11.91
    ATOM 1577 C   PRO A 206 0   2.739 27.411 23.045 1.00 14.01
    ATOM 1578 O   PRO A 206 0   3.676 28.135 22.661 1.00 14.38
 30 ATOM 1579 CB  PRO A 206 0   1.124 26.816 21.262 1.00 11.87
    ATOM 1580 CG  PRO A 206 0   1.112 27.893 20.191 1.00 12.83
    ATOM 1581 CD  PRO A 206 0   0.749 29.241 20.766 1.00 11.09
    ATOM 1582 N   ASN A 207 0   2.888 26.439 23.911 1.00 13.06
    ATOM 1583 CA  ASN A 207 0   4.128 25.919 24.429 1.00 15.01
 35 ATOM 1584 C   ASN A 207 0   4.332 24.591 23.677 1.00 15.84
    ATOM 1585 O   ASN A 207 0   3.376 24.095 23.038 1.00 16.22
    ATOM 1586 CB  ASN A 207 0   4.144 25.682 25.933 1.00 15.12
    ATOM 1587 CG  ASN A 207 0   3.054 24.708 26.395 1.00 19.36
```

```
    ATOM   1588  OD1 ASN A 207  0    2.062 25.161 27.014  1.00 19.36
    ATOM   1589  ND2 ASN A 207  0    3.174 23.408 26.203  1.00 16.49
    ATOM   1590  N   TRP A 208  0    5.557 24.077 23.634  1.00 14.46
    ATOM   1591  CA  TRP A 208  0    5.827 22.865 22.892  1.00 12.04
  5 ATOM   1592  C   TRP A 208  0    6.638 21.921 23.783  1.00 13.85
    ATOM   1593  O   TRP A 208  0    7.482 22.385 24.558  1.00 13.02
    ATOM   1594  CB  TRP A 208  0    6.654 23.136 21.628  1.00 11.91
    ATOM   1595  CG  TRP A 208  0    5.951 23.769 20.465  1.00 11.27
    ATOM   1596  CD1 TRP A 208  0    5.149 23.164 19.561  1.00 10.33
 10 ATOM   1597  CD2 TRP A 208  0    5.988 25.158 20.092  1.00 10.29
    ATOM   1598  NE1 TRP A 208  0    4.698 24.078 18.625  1.00 10.91
    ATOM   1599  CE2 TRP A 208  0    5.201 25.313 18.954  1.00  9.64
    ATOM   1600  CE3 TRP A 208  0    6.634 26.294 20.625  1.00 10.25
    ATOM   1601  CZ2 TRP A 208  0    5.011 26.553 18.344  1.00  8.53
 15 ATOM   1602  CZ3 TRP A 208  0    6.494 27.514 20.019  1.00 10.02
    ATOM   1603  CH2 TRP A 208  0    5.668 27.633 18.881  1.00 11.79
    ATOM   1604  N   GLN A 209  0    6.420 20.620 23.580  1.00 13.82
    ATOM   1605  CA  GLN A 209  0    7.240 19.588 24.192  1.00 13.83
    ATOM   1606  C   GLN A 209  0    8.251 19.281 23.075  1.00 13.07
 20 ATOM   1607  O   GLN A 209  0    7.848 18.968 21.948  1.00 14.18
    ATOM   1608  CB  GLN A 209  0    6.441 18.319 24.487  1.00 15.65
    ATOM   1609  CG  GLN A 209  0    5.449 18.481 25.649  1.00 17.26
    ATOM   1610  CD  GLN A 209  0    6.177 18.514 26.975  1.00 18.17
    ATOM   1611  OE1 GLN A 209  0    7.414 18.471 27.002  1.00 20.00
 25 ATOM   1612  NE2 GLN A 209  0    5.462 18.570 28.085  1.00 16.89
    ATOM   1613  N   PHE A 210  0    9.538 19.461 23.351  1.00 11.26
    ATOM   1614  CA  PHE A 210  0   10.526 19.329 22.287  1.00 10.01
    ATOM   1615  C   PHE A 210  0   11.457 18.153 22.585  1.00  9.18
    ATOM   1616  O   PHE A 210  0   11.894 17.999 23.732  1.00 10.07
 30 ATOM   1617  CB  PHE A 210  0   11.370 20.629 22.292  1.00 10.86
    ATOM   1618  CG  PHE A 210  0   12.489 20.581 21.292  1.00  9.63
    ATOM   1619  CD1 PHE A 210  0   13.760 20.179 21.674  1.00  9.95
    ATOM   1620  CD2 PHE A 210  0   12.251 20.922 19.984  1.00  8.54
    ATOM   1621  CE1 PHE A 210  0   14.778 20.150 20.738  1.00  9.23
 35 ATOM   1622  CE2 PHE A 210  0   13.243 20.862 19.023  1.00  7.93
    ATOM   1623  CZ  PHE A 210  0   14.520 20.491 19.426  1.00  8.71
    ATOM   1624  N   SER A 211  0   11.741 17.384 21.545  1.00  8.62
    ATOM   1625  CA  SER A 211  0   12.645 16.255 21.716  1.00 10.71
```

```
    ATOM   1626 C   SER A 211 0   13.142 15.844 20.347 1.00 11.36
    ATOM   1627 O   SER A 211 0   12.661 16.323 19.315 1.00 9.99
    ATOM   1628 CB  SER A 211 0   11.970 15.070 22.427 1.00 10.56
    ATOM   1629 OG  SER A 211 0   10.899 14.731 21.513 1.00 12.92
 5  ATOM   1630 N   ILE A 212 0   14.268 15.122 20.390 1.00 13.67
    ATOM   1631 CA  ILE A 212 0   14.883 14.680 19.131 1.00 14.79
    ATOM   1632 C   ILE A 212 0   15.013 13.166 19.220 1.00 15.44
    ATOM   1633 O   ILE A 212 0   15.624 12.689 20.177 1.00 15.98
    ATOM   1634 CB  ILE A 212 0   16.255 15.341 18.887 1.00 17.04
10  ATOM   1635 CG1 ILE A 212 0   16.082 16.859 18.756 1.00 15.64
    ATOM   1636 CG2 ILE A 212 0   16.935 14.722 17.648 1.00 15.24
    ATOM   1637 CD1 ILE A 212 0   17.352 17.648 18.553 1.00 16.57
    ATOM   1638 N   ASP A 213 0   14.453 12.418 18.281 1.00 15.53
    ATOM   1639 CA  ASP A 213 0   14.549 10.952 18.401 1.00 16.50
15  ATOM   1640 C   ASP A 213 0   16.004 10.469 18.541 1.00 16.69
    ATOM   1641 O   ASP A 213 0   16.948 10.902 17.851 1.00 14.36
    ATOM   1642 CB  ASP A 213 0   13.884 10.359 17.173 1.00 17.15
    ATOM   1643 CG  ASP A 213 0   12.369 10.467 17.144 1.00 18.12
    ATOM   1644 OD1 ASP A 213 0   11.751 10.995 18.092 1.00 16.90
20  ATOM   1645 OD2 ASP A 213 0   11.801  9.990 16.129 1.00 17.35
    ATOM   1646 N   GLY A 214 0   16.198  9.559 19.477 1.00 15.76
    ATOM   1647 CA  GLY A 214 0   17.457  8.900 19.747 1.00 17.22
    ATOM   1648 C   GLY A 214 0   18.548  9.757 20.368 1.00 18.54
    ATOM   1649 O   GLY A 214 0   19.680  9.277 20.404 1.00 18.20
25  ATOM   1650 N   HIS A 215 0   18.341 11.024 20.738 1.00 18.17
    ATOM   1651 CA  HIS A 215 0   19.422 11.880 21.229 1.00 17.59
    ATOM   1652 C   HIS A 215 0   19.096 12.505 22.577 1.00 17.92
    ATOM   1653 O   HIS A 215 0   17.917 12.696 22.898 1.00 20.45
    ATOM   1654 CB  HIS A 215 0   19.705 13.008 20.221 1.00 15.73
30  ATOM   1655 CG  HIS A 215 0   20.309 12.543 18.936 1.00 16.90
    ATOM   1656 ND1 HIS A 215 0   19.589 11.864 17.963 1.00 17.35
    ATOM   1657 CD2 HIS A 215 0   21.574 12.658 18.444 1.00 16.15
    ATOM   1658 CE1 HIS A 215 0   20.376 11.576 16.933 1.00 17.63
    ATOM   1659 NE2 HIS A 215 0   21.599 12.046 17.216 1.00 17.73
35  ATOM   1660 N   GLU A 216 0   20.104 12.815 23.382 1.00 17.22
    ATOM   1661 CA  GLU A 216 0   19.876 13.479 24.665 1.00 15.86
    ATOM   1662 C   GLU A 216 0   20.070 14.976 24.456 1.00 15.61
    ATOM   1663 O   GLU A 216 0   20.684 15.386 23.453 1.00 14.96
```

```
     ATOM  1664 CB  GLU A 216 0  20.817 12.901 25.694 1.00 15.38
     ATOM  1665 CG  GLU A 216 0  20.440 11.520 26.166 1.00 16.53
     ATOM  1666 CD  GLU A 216 0  21.242 11.058 27.357 1.00 17.23
     ATOM  1667 OE1 GLU A 216 0  22.378 10.619 27.129 1.00 20.31
   5 ATOM  1668 OE2 GLU A 216 0  20.813 11.119 28.519 1.00 16.06
     ATOM  1669 N   LEU A 217 0  19.623 15.792 25.394 1.00 14.64
     ATOM  1670 CA  LEU A 217 0  19.738 17.243 25.251 1.00 14.91
     ATOM  1671 C   LEU A 217 0  20.512 17.792 26.446 1.00 14.71
     ATOM  1672 O   LEU A 217 0  19.950 17.734 27.539 1.00 15.67
  10 ATOM  1673 CB  LEU A 217 0  18.362 17.931 25.229 1.00 14.75
     ATOM  1674 CG  LEU A 217 0  17.276 17.349 24.306 1.00 15.40
     ATOM  1675 CD1 LEU A 217 0  15.939 18.075 24.505 1.00 15.08
     ATOM  1676 CD2 LEU A 217 0  17.723 17.453 22.849 1.00 15.22
     ATOM  1677 N   THR A 218 0  21.732 18.278 26.229 1.00 13.65
  15 ATOM  1678 CA  THR A 218 0  22.507 18.714 27.402 1.00 13.26
     ATOM  1679 C   THR A 218 0  22.427 20.232 27.505 1.00 13.27
     ATOM  1680 O   THR A 218 0  23.142 20.955 26.805 1.00 12.91
     ATOM  1681 CB  THR A 218 0  23.955 18.216 27.304 1.00 12.08
     ATOM  1682 OG1 THR A 218 0  23.935 16.782 27.331 1.00 15.48
  20 ATOM  1683 CG2 THR A 218 0  24.767 18.721 28.470 1.00 11.46
     ATOM  1684 N   ILE A 219 0  21.522 20.649 28.385 1.00 13.30
     ATOM  1685 CA  ILE A 219 0  21.259 22.068 28.547 1.00 14.53
     ATOM  1686 C   ILE A 219 0  22.420 22.818 29.180 1.00 12.72
     ATOM  1687 O   ILE A 219 0  22.795 22.492 30.292 1.00 13.08
  25 ATOM  1688 CB  ILE A 219 0  19.930 22.268 29.323 1.00 14.74
     ATOM  1689 CG1 ILE A 219 0  18.761 21.699 28.441 1.00 17.33
     ATOM  1690 CG2 ILE A 219 0  19.666 23.717 29.656 1.00 13.40
     ATOM  1691 CD1 ILE A 219 0  17.597 21.481 29.412 1.00 19.42
     ATOM  1692 N   ILE A 220 0  22.898 23.869 28.510 1.00 12.55
  30 ATOM  1693 CA  ILE A 220 0  23.994 24.696 29.019 1.00 13.25
     ATOM  1694 C   ILE A 220 0  23.686 26.193 29.085 1.00 15.11
     ATOM  1695 O   ILE A 220 0  24.477 27.001 29.618 1.00 14.73
     ATOM  1696 CB  ILE A 220 0  25.239 24.507 28.125 1.00 11.80
     ATOM  1697 CG1 ILE A 220 0  24.954 24.871 26.671 1.00 10.93
  35 ATOM  1698 CG2 ILE A 220 0  25.770 23.072 28.291 1.00  9.59
     ATOM  1699 CD1 ILE A 220 0  26.249 25.231 25.928 1.00 12.07
     ATOM  1700 N   GLU A 221 0  22.490 26.573 28.597 1.00 13.30
     ATOM  1701 CA  GLU A 221 0  22.048 27.951 28.624 1.00 12.96
```

```
   ATOM  1702 C   GLU A 221  0   20.522 28.066 28.727 1.00 13.77
   ATOM  1703 O   GLU A 221  0   19.799 27.301 28.068 1.00 14.06
   ATOM  1704 CB  GLU A 221  0   22.436 28.666 27.318 1.00 12.73
   ATOM  1705 CG  GLU A 221  0   22.280 30.178 27.325 1.00 12.94
 5 ATOM  1706 CD  GLU A 221  0   22.018 30.783 25.969 1.00 13.84
   ATOM  1707 OE1 GLU A 221  0   22.345 30.269 24.887 1.00 12.66
   ATOM  1708 OE2 GLU A 221  0   21.386 31.862 25.936 1.00 14.80
   ATOM  1709 N   VAL A 222  0   20.062 29.091 29.434 1.00 13.89
   ATOM  1710 CA  VAL A 222  0   18.632 29.350 29.534 1.00 14.13
10 ATOM  1711 C   VAL A 222  0   18.409 30.853 29.493 1.00 13.87
   ATOM  1712 O   VAL A 222  0   18.900 31.657 30.300 1.00 11.55
   ATOM  1713 CB  VAL A 222  0   18.003 28.649 30.737 1.00 16.86
   ATOM  1714 CG1 VAL A 222  0   18.730 28.941 32.017 1.00 19.16
   ATOM  1715 CG2 VAL A 222  0   16.575 29.120 31.033 1.00 18.45
15 ATOM  1716 N   ASP A 223  0   17.631 31.267 28.481 1.00 11.69
   ATOM  1717 CA  ASP A 223  0   17.245 32.673 28.386 1.00 13.60
   ATOM  1718 C   ASP A 223  0   18.472 33.598 28.548 1.00 14.44
   ATOM  1719 O   ASP A 223  0   18.423 34.552 29.336 1.00 12.75
   ATOM  1720 CB  ASP A 223  0   16.161 33.033 29.417 1.00 12.59
20 ATOM  1721 CG  ASP A 223  0   14.845 32.279 29.364 1.00 14.64
   ATOM  1722 OD1 ASP A 223  0   14.697 31.397 28.493 1.00 13.34
   ATOM  1723 OD2 ASP A 223  0   13.858 32.463 30.156 1.00 13.85
   ATOM  1724 N   GLY A 224  0   19.544 33.372 27.767 1.00 13.49
   ATOM  1725 CA  GLY A 224  0   20.728 34.213 27.770 1.00 12.85
25 ATOM  1726 C   GLY A 224  0   21.562 34.112 29.049 1.00 13.00
   ATOM  1727 O   GLY A 224  0   22.326 35.040 29.317 1.00 13.97
   ATOM  1728 N   GLU A 225  0   21.370 33.105 29.875 1.00 11.78
   ATOM  1729 CA  GLU A 225  0   22.068 32.888 31.114 1.00 14.97
   ATOM  1730 C   GLU A 225  0   22.609 31.447 31.106 1.00 16.73
30 ATOM  1731 O   GLU A 225  0   21.858 30.498 30.849 1.00 15.88
   ATOM  1732 CB  GLU A 225  0   21.174 33.062 32.358 1.00 16.54
   ATOM  1733 CG  GLU A 225  0   20.509 34.424 32.534 1.00 16.30
   ATOM  1734 CD  GLU A 225  0   21.492 35.546 32.823 1.00 17.57
   ATOM  1735 OE1 GLU A 225  0   22.450 35.254 33.561 1.00 18.76
35 ATOM  1736 OE2 GLU A 225  0   21.360 36.711 32.360 1.00 17.77
   ATOM  1737 N   LEU A 226  0   23.922 31.285 31.324 1.00 16.90
   ATOM  1738 CA  LEU A 226  0   24.526 29.955 31.318 1.00 15.50
   ATOM  1739 C   LEU A 226  0   24.183 29.127 32.540 1.00 15.04
```

```
  ATOM 1740 O   LEU A 226 0  24.002 29.648 33.652 1.00 15.17
  ATOM 1741 CB  LEU A 226 0  26.062 30.008 31.216 1.00 15.36
  ATOM 1742 CG  LEU A 226 0  26.567 30.741 29.958 1.00 17.95
  ATOM 1743 CD1 LEU A 226 0  28.076 30.876 29.979 1.00 18.77
5 ATOM 1744 CD2 LEU A 226 0  26.111 30.029 28.687 1.00 17.36
  ATOM 1745 N   THR A 227 0  24.119 27.799 32.332 1.00 13.62
  ATOM 1746 CA  THR A 227 0  23.848 26.930 33.479 1.00 13.72
  ATOM 1747 C   THR A 227 0  24.936 25.851 33.528 1.00 14.30
  ATOM 1748 O   THR A 227 0  25.732 25.629 32.592 1.00 14.28
10 ATOM 1749 CB  THR A 227 0  22.478 26.217 33.352 1.00 14.35
  ATOM 1750 OG1 THR A 227 0  22.506 25.385 32.178 1.00 13.68
  ATOM 1751 CG2 THR A 227 0  21.284 27.161 33.180 1.00 12.29
  ATOM 1752 N   GLU A 228 0  24.960 25.136 34.625 1.00 14.73
  ATOM 1753 CA  GLU A 228 0  25.765 23.907 34.714 1.00 17.32
15 ATOM 1754 C   GLU A 228 0  25.110 22.971 33.680 1.00 17.30
  ATOM 1755 O   GLU A 228 0  23.917 23.035 33.472 1.00 16.97
  ATOM 1756 CB  GLU A 228 0  25.617 23.315 36.114 1.00 16.58
  ATOM 1757 CG  GLU A 228 0  26.493 23.979 37.186 1.00 18.10
  ATOM 1758 CD  GLU A 228 0  26.236 23.458 38.575 1.00 20.92
20 ATOM 1759 OE1 GLU A 228 0  25.469 22.470 38.755 1.00 23.38
  ATOM 1760 OE2 GLU A 228 0  26.769 23.997 39.564 1.00 21.26
  ATOM 1761 N   PRO A 229 0  25.867 22.158 32.984 1.00 16.91
  ATOM 1762 CA  PRO A 229 0  25.369 21.207 31.992 1.00 16.37
  ATOM 1763 C   PRO A 229 0  24.351 20.275 32.599 1.00 16.24
25 ATOM 1764 O   PRO A 229 0  24.624 19.652 33.619 1.00 15.76
  ATOM 1765 CB  PRO A 229 0  26.612 20.469 31.419 1.00 15.97
  ATOM 1766 CG  PRO A 229 0  27.701 21.509 31.741 1.00 15.92
  ATOM 1767 CD  PRO A 229 0  27.337 22.141 33.083 1.00 14.86
  ATOM 1768 N   HIS A 230 0  23.140 20.164 32.038 1.00 15.58
30 ATOM 1769 CA  HIS A 230 0  22.090 19.325 32.618 1.00 15.01
  ATOM 1770 C   HIS A 230 0  21.354 18.610 31.488 1.00 13.55
  ATOM 1771 O   HIS A 230 0  20.756 19.192 30.590 1.00 13.47
  ATOM 1772 CB  HIS A 230 0  21.172 20.164 33.510 1.00 15.89
  ATOM 1773 CG  HIS A 230 0  20.045 19.341 34.064 1.00 18.32
35 ATOM 1774 ND1 HIS A 230 0  20.252 18.347 35.004 1.00 18.14
  ATOM 1775 CD2 HIS A 230 0  18.713 19.328 33.791 1.00 17.75
  ATOM 1776 CE1 HIS A 230 0  19.121 17.768 35.310 1.00 16.33
  ATOM 1777 NE2 HIS A 230 0  18.173 18.344 34.609 1.00 17.85
```

```
     ATOM  1778 N   THR A 231 0  21.496 17.304 31.458 1.00 12.94
     ATOM  1779 CA  THR A 231 0  20.995 16.474 30.346 1.00 14.15
     ATOM  1780 C   THR A 231 0  19.620 15.890 30.547 1.00 13.41
     ATOM  1781 O   THR A 231 0  19.293 15.401 31.616 1.00 14.89
   5 ATOM  1782 CB  THR A 231 0  22.040 15.364 30.060 1.00 13.73
     ATOM  1783 OG1 THR A 231 0  23.314 16.023 29.852 1.00 14.77
     ATOM  1784 CG2 THR A 231 0  21.655 14.600 28.818 1.00 13.06
     ATOM  1785 N   VAL A 232 0  18.776 15.954 29.549 1.00 12.86
     ATOM  1786 CA  VAL A 232 0  17.374 15.505 29.665 1.00 13.44
  10 ATOM  1787 C   VAL A 232 0  16.999 14.966 28.319 1.00 14.96
     ATOM  1788 O   VAL A 232 0  17.790 15.258 27.390 1.00 14.12
     ATOM  1789 CB  VAL A 232 0  16.771 16.910 30.000 1.00 17.41
     ATOM  1790 CG1 VAL A 232 0  16.075 17.587 28.856 1.00 14.66
     ATOM  1791 CG2 VAL A 232 0  16.158 16.935 31.371 1.00 15.66
  15 ATOM  1792 N   ASP A 233 0  15.874 14.277 28.153 1.00 14.01
     ATOM  1793 CA  ASP A 233 0  15.405 13.803 26.874 1.00 14.73
     ATOM  1794 C   ASP A 233 0  14.353 14.718 26.245 1.00 14.74
     ATOM  1795 O   ASP A 233 0  14.187 14.731 25.027 1.00 13.41
     ATOM  1796 CB  ASP A 233 0  14.640 12.465 27.046 1.00 16.54
  20 ATOM  1797 CG  ASP A 233 0  15.637 11.417 27.536 1.00 19.27
     ATOM  1798 OD1 ASP A 233 0  16.543 11.145 26.732 1.00 20.98
     ATOM  1799 OD2 ASP A 233 0  15.536 10.945 28.667 1.00 19.27
     ATOM  1800 N   ARG A 234 0  13.595 15.386 27.122 1.00 13.79
     ATOM  1801 CA  ARG A 234 0  12.514 16.199 26.598 1.00 16.36
  25 ATOM  1802 C   ARG A 234 0  12.258 17.426 27.472 1.00 15.17
     ATOM  1803 O   ARG A 234 0  12.418 17.390 28.686 1.00 13.96
     ATOM  1804 CB  ARG A 234 0  11.265 15.330 26.482 1.00 19.23
     ATOM  1805 CG  ARG A 234 0  10.104 16.036 25.788 1.00 22.25
     ATOM  1806 CD  ARG A 234 0   8.981 15.023 25.506 1.00 24.68
  30 ATOM  1807 NE  ARG A 234 0   8.157 14.983 26.705 1.00 28.27
     ATOM  1808 CZ  ARG A 234 0   6.845 14.828 26.719 1.00 28.66
     ATOM  1809 NH1 ARG A 234 0   6.291 14.833 27.909 1.00 30.08
     ATOM  1810 NH2 ARG A 234 0   6.191 14.662 25.587 1.00 30.24
     ATOM  1811 N   LEU A 235 0  11.874 18.524 26.816 1.00 13.90
  35 ATOM  1812 CA  LEU A 235 0  11.619 19.742 27.607 1.00 13.15
     ATOM  1813 C   LEU A 235 0  10.390 20.430 27.041 1.00 11.49
     ATOM  1814 O   LEU A 235 0  10.025 20.304 25.873 1.00 11.08
     ATOM  1815 CB  LEU A 235 0  12.825 20.630 27.695 1.00 14.39
```

```
   ATOM  1816 CG  LEU A 235 0  13.459 21.645 26.801 1.00 17.19
   ATOM  1817 CD1 LEU A 235 0  14.795 21.218 26.197 1.00 16.98
   ATOM  1818 CD2 LEU A 235 0  12.586 22.219 25.685 1.00 18.24
   ATOM  1819 N   GLN A 236 0   9.769 21.152 27.949 1.00 12.74
 5 ATOM  1820 CA  GLN A 236 0   8.576 21.944 27.616 1.00 13.45
   ATOM  1821 C   GLN A 236 0   9.005 23.390 27.459 1.00 12.21
   ATOM  1822 O   GLN A 236 0   9.606 23.939 28.406 1.00 13.90
   ATOM  1823 CB  GLN A 236 0   7.525 21.770 28.741 1.00 12.06
   ATOM  1824 CG  GLN A 236 0   6.197 22.276 28.238 1.00 14.12
10 ATOM  1825 CD  GLN A 236 0   5.025 22.108 29.205 1.00 13.35
   ATOM  1826 OE1 GLN A 236 0   3.893 22.215 28.721 1.00 15.61
   ATOM  1827 NE2 GLN A 236 0   5.226 21.912 30.463 1.00 12.00
   ATOM  1828 N   ILE A 237 0   8.748 24.011 26.311 1.00 12.17
   ATOM  1829 CA  ILE A 237 0   9.213 25.390 26.156 1.00 12.41
15 ATOM  1830 C   ILE A 237 0   8.061 26.376 25.953 1.00 13.14
   ATOM  1831 O   ILE A 237 0   7.283 26.310 24.990 1.00 13.64
   ATOM  1832 CB  ILE A 237 0  10.255 25.437 25.022 1.00 11.03
   ATOM  1833 CG1 ILE A 237 0  10.947 26.793 24.960 1.00 11.84
   ATOM  1834 CG2 ILE A 237 0   9.615 25.086 23.662 1.00 10.02
20 ATOM  1835 CD1 ILE A 237 0  12.041 26.953 23.902 1.00 11.23
   ATOM  1836 N   PHE A 238 0   8.037 27.414 26.765 1.00 12.83
   ATOM  1837 CA  PHE A 238 0   6.979 28.431 26.714 1.00 13.23
   ATOM  1838 C   PHE A 238 0   7.382 29.683 25.957 1.00 13.99
   ATOM  1839 O   PHE A 238 0   8.530 29.848 25.545 1.00 13.87
25 ATOM  1840 CB  PHE A 238 0   6.592 28.848 28.145 1.00 12.72
   ATOM  1841 CG  PHE A 238 0   6.176 27.691 28.993 1.00 14.51
   ATOM  1842 CD1 PHE A 238 0   7.098 26.957 29.710 1.00 14.84
   ATOM  1843 CD2 PHE A 238 0   4.836 27.314 29.078 1.00 15.50
   ATOM  1844 CE1 PHE A 238 0   6.748 25.882 30.497 1.00 13.87
30 ATOM  1845 CE2 PHE A 238 0   4.468 26.236 29.862 1.00 14.62
   ATOM  1846 CZ  PHE A 238 0   5.423 25.528 30.568 1.00 15.15
   ATOM  1847 N   THR A 239 0   6.388 30.494 25.604 1.00 14.16
   ATOM  1848 CA  THR A 239 0   6.543 31.678 24.806 1.00 13.44
   ATOM  1849 C   THR A 239 0   7.832 32.453 25.106 1.00 11.74
35 ATOM  1850 O   THR A 239 0   8.012 32.950 26.218 1.00 10.47
   ATOM  1851 CB  THR A 239 0   5.381 32.695 24.978 1.00 15.55
   ATOM  1852 OG1 THR A 239 0   5.258 33.008 26.359 1.00 17.88
   ATOM  1853 CG2 THR A 239 0   4.055 32.131 24.478 1.00 16.75
```

```
   ATOM   1854 N   GLY A 240  0    8.672 32.593 24.078 1.00  7.94
   ATOM   1855 CA  GLY A 240  0    9.877 33.348 24.193 1.00 10.08
   ATOM   1856 C   GLY A 240  0   11.039 32.865 25.041 1.00 11.34
   ATOM   1857 O   GLY A 240  0   11.977 33.650 25.216 1.00 11.02
 5 ATOM   1858 N   GLN A 241  0   10.990 31.646 25.592 1.00  9.73
   ATOM   1859 CA  GLN A 241  0   12.067 31.090 26.364 1.00  9.59
   ATOM   1860 C   GLN A 241  0   13.114 30.587 25.342 1.00 10.56
   ATOM   1861 O   GLN A 241  0   12.823 30.467 24.126 1.00  8.44
   ATOM   1862 CB  GLN A 241  0   11.604 29.965 27.285 1.00 10.57
10 ATOM   1863 CG  GLN A 241  0   10.820 30.363 28.523 1.00 10.54
   ATOM   1864 CD  GLN A 241  0   10.341 29.190 29.341 1.00 12.22
   ATOM   1865 OE1 GLN A 241  0   10.118 28.077 28.815 1.00 13.21
   ATOM   1866 NE2 GLN A 241  0   10.220 29.466 30.639 1.00 11.74
   ATOM   1867 N   ARG A 242  0   14.372 30.492 25.774 1.00  9.00
15 ATOM   1868 CA  ARG A 242  0   15.388 29.992 24.834 1.00 11.01
   ATOM   1869 C   ARG A 242  0   16.210 28.966 25.609 1.00 11.30
   ATOM   1870 O   ARG A 242  0   16.292 29.133 26.816 1.00  9.51
   ATOM   1871 CB  ARG A 242  0   16.324 31.043 24.265 1.00 12.77
   ATOM   1872 CG  ARG A 242  0   15.694 32.128 23.364 1.00 12.52
20 ATOM   1873 CD  ARG A 242  0   15.066 33.249 24.138 1.00 10.81
   ATOM   1874 NE  ARG A 242  0   15.957 34.126 24.892 1.00 10.80
   ATOM   1875 CZ  ARG A 242  0   15.630 34.761 26.002 1.00 11.36
   ATOM   1876 NH1 ARG A 242  0   16.486 35.548 26.648 1.00  7.98
   ATOM   1877 NH2 ARG A 242  0   14.365 34.589 26.489 1.00 12.78
25 ATOM   1878 N   TYR A 243  0   16.717 27.934 24.942 1.00 11.61
   ATOM   1879 CA  TYR A 243  0   17.631 27.009 25.610 1.00 12.54
   ATOM   1880 C   TYR A 243  0   18.819 26.762 24.650 1.00 14.46
   ATOM   1881 O   TYR A 243  0   18.568 26.656 23.435 1.00 16.11
   ATOM   1882 CB  TYR A 243  0   17.015 25.638 25.934 1.00 11.09
30 ATOM   1883 CG  TYR A 243  0   16.007 25.667 27.054 1.00 12.11
   ATOM   1884 CD1 TYR A 243  0   14.641 25.825 26.843 1.00 12.88
   ATOM   1885 CD2 TYR A 243  0   16.440 25.575 28.371 1.00 12.11
   ATOM   1886 CE1 TYR A 243  0   13.748 25.869 27.915 1.00 12.71
   ATOM   1887 CE2 TYR A 243  0   15.560 25.582 29.436 1.00 12.50
35 ATOM   1888 CZ  TYR A 243  0   14.205 25.738 29.188 1.00 12.29
   ATOM   1889 OH  TYR A 243  0   13.379 25.789 30.286 1.00 13.65
   ATOM   1890 N   SER A 244  0   20.059 26.734 25.144 1.00 12.78
   ATOM   1891 CA  SER A 244  0   21.117 26.212 24.268 1.00 13.22
```

```
   ATOM 1892 C   SER A 244  0  21.333 24.779 24.814 1.00 11.06
   ATOM 1893 O   SER A 244  0  21.377 24.604 26.018 1.00 11.27
   ATOM 1894 CB  SER A 244  0  22.485 26.907 24.308 1.00 14.46
   ATOM 1895 OG  SER A 244  0  22.551 28.029 23.463 1.00 13.59
 5 ATOM 1896 N   PHE A 245  0  21.484 23.780 23.983 1.00 11.89
   ATOM 1897 CA  PHE A 245  0  21.772 22.437 24.452 1.00 13.14
   ATOM 1898 C   PHE A 245  0  22.867 21.857 23.546 1.00 12.32
   ATOM 1899 O   PHE A 245  0  22.890 22.128 22.354 1.00 11.11
   ATOM 1900 CB  PHE A 245  0  20.554 21.495 24.526 1.00 11.40
10 ATOM 1901 CG  PHE A 245  0  19.915 21.236 23.195 1.00 11.98
   ATOM 1902 CD1 PHE A 245  0  18.815 21.993 22.813 1.00 13.38
   ATOM 1903 CD2 PHE A 245  0  20.349 20.236 22.351 1.00 11.45
   ATOM 1904 CE1 PHE A 245  0  18.216 21.773 21.588 1.00 12.84
   ATOM 1905 CE2 PHE A 245  0  19.759 20.000 21.129 1.00 11.48
15 ATOM 1906 CZ  PHE A 245  0  18.705 20.796 20.743 1.00 12.65
   ATOM 1907 N   VAL A 246  0  23.742 21.073 24.169 1.00 13.51
   ATOM 1908 CA  VAL A 246  0  24.775 20.427 23.341 1.00 13.37
   ATOM 1909 C   VAL A 246  0  24.096 19.177 22.783 1.00 12.47
   ATOM 1910 O   VAL A 246  0  23.505 18.425 23.540 1.00 11.41
20 ATOM 1911 CB  VAL A 246  0  25.990 19.984 24.190 1.00 14.96
   ATOM 1912 CG1 VAL A 246  0  26.995 19.186 23.364 1.00 13.75
   ATOM 1913 CG2 VAL A 246  0  26.681 21.165 24.841 1.00 15.92
   ATOM 1914 N   LEU A 247  0  24.160 18.996 21.490 1.00 12.97
   ATOM 1915 CA  LEU A 247  0  23.766 17.833 20.785 1.00 14.32
25 ATOM 1916 C   LEU A 247  0  25.071 17.077 20.395 1.00 14.22
   ATOM 1917 O   LEU A 247  0  25.954 17.529 19.664 1.00 12.45
   ATOM 1918 CB  LEU A 247  0  22.980 18.109 19.505 1.00 16.00
   ATOM 1919 CG  LEU A 247  0  22.514 16.786 18.835 1.00 16.80
   ATOM 1920 CD1 LEU A 247  0  21.266 16.306 19.513 1.00 18.30
30 ATOM 1921 CD2 LEU A 247  0  22.207 16.988 17.373 1.00 18.70
   ATOM 1922 N   ASP A 248  0  25.144 15.886 20.926 1.00 13.56
   ATOM 1923 CA  ASP A 248  0  26.278 14.980 20.727 1.00 16.65
   ATOM 1924 C   ASP A 248  0  25.916 14.072 19.581 1.00 16.18
   ATOM 1925 O   ASP A 248  0  25.095 13.166 19.813 1.00 17.60
35 ATOM 1926 CB  ASP A 248  0  26.536 14.229 22.036 1.00 17.83
   ATOM 1927 CG  ASP A 248  0  27.798 13.359 22.024 1.00 21.77
   ATOM 1928 OD1 ASP A 248  0  28.231 12.967 23.140 1.00 24.11
   ATOM 1929 OD2 ASP A 248  0  28.345 13.060 20.950 1.00 21.25
```

```
  ATOM 1930 N   ALA A 249 0  26.414 14.277 18.369 1.00 15.85
  ATOM 1931 CA  ALA A 249 0  25.982 13.416 17.255 1.00 17.99
  ATOM 1932 C   ALA A 249 0  26.698 12.049 17.306 1.00 20.21
  ATOM 1933 O   ALA A 249 0  27.569 11.766 16.485 1.00 19.11
5 ATOM 1934 CB  ALA A 249 0  26.165 14.126 15.930 1.00 14.57
  ATOM 1935 N   ASN A 250 0  26.273 11.223 18.253 1.00 21.66
  ATOM 1936 CA  ASN A 250 0  26.861  9.961 18.581 1.00 25.53
  ATOM 1937 C   ASN A 250 0  26.061  8.721 18.202 1.00 27.30
  ATOM 1938 O   ASN A 250 0  26.344  7.645 18.756 1.00 29.42
10 ATOM 1939 CB  ASN A 250 0  27.108  9.912 20.104 1.00 25.83
  ATOM 1940 CG  ASN A 250 0  25.888  9.968 20.978 1.00 28.76
  ATOM 1941 OD1 ASN A 250 0  24.757 10.156 20.527 1.00 29.90
  ATOM 1942 ND2 ASN A 250 0  26.042  9.826 22.306 1.00 29.52
  ATOM 1943 N   GLN A 251 0  25.089  8.841 17.302 1.00 26.74
15 ATOM 1944 CA  GLN A 251 0  24.239  7.712 16.934 1.00 23.48
  ATOM 1945 C   GLN A 251 0  24.583  7.311 15.510 1.00 21.73
  ATOM 1946 O   GLN A 251 0  25.333  8.009 14.843 1.00 19.39
  ATOM 1947 CB  GLN A 251 0  22.757  8.104 17.022 1.00 24.79
  ATOM 1948 CG  GLN A 251 0  22.333  8.701 18.360 1.00 25.14
20 ATOM 1949 CD  GLN A 251 0  22.430  7.693 19.480 1.00 26.76
  ATOM 1950 OE1 GLN A 251 0  21.762  6.654 19.405 1.00 28.78
  ATOM 1951 NE2 GLN A 251 0  23.202  7.986 20.514 1.00 26.02
  ATOM 1952 N   PRO A 252 0  24.058  6.177 15.076 1.00 20.53
  ATOM 1953 CA  PRO A 252 0  24.293  5.637 13.755 1.00 20.06
25 ATOM 1954 C   PRO A 252 0  23.940  6.671 12.702 1.00 21.83
  ATOM 1955 O   PRO A 252 0  22.973  7.424 12.940 1.00 22.51
  ATOM 1956 CB  PRO A 252 0  23.417  4.367 13.647 1.00 19.98
  ATOM 1957 CG  PRO A 252 0  23.288  3.997 15.096 1.00 19.94
  ATOM 1958 CD  PRO A 252 0  23.223  5.289 15.902 1.00 19.68
30 ATOM 1959 N   VAL A 253 0  24.663  6.728 11.584 1.00 20.85
  ATOM 1960 CA  VAL A 253 0  24.302  7.741 10.604 1.00 22.29
  ATOM 1961 C   VAL A 253 0  22.897  7.414 10.108 1.00 23.02
  ATOM 1962 O   VAL A 253 0  22.593  6.289  9.753 1.00 21.37
  ATOM 1963 CB  VAL A 253 0  25.298  8.065  9.494 1.00 23.22
35 ATOM 1964 CG1 VAL A 253 0  26.696  7.582  9.827 1.00 22.25
  ATOM 1965 CG2 VAL A 253 0  24.859  7.680  8.101 1.00 22.26
  ATOM 1966 N   ASP A 254 0  22.012  8.422 10.159 1.00 24.32
  ATOM 1967 CA  ASP A 254 0  20.613  8.176  9.786 1.00 22.09
```

```
   ATOM  1968  C   ASP A 254  0   19.782   9.448   9.821  1.00 20.71
   ATOM  1969  O   ASP A 254  0   20.365  10.481  10.099  1.00 18.92
   ATOM  1970  CB  ASP A 254  0   20.048   7.211  10.830  1.00 23.39
   ATOM  1971  CG  ASP A 254  0   18.964   6.331  10.251  1.00 24.43
 5 ATOM  1972  OD1 ASP A 254  0   18.355   6.663   9.239  1.00 23.21
   ATOM  1973  OD2 ASP A 254  0   18.736   5.244  10.816  1.00 28.26
   ATOM  1974  N   ASN A 255  0   18.485   9.338   9.496  1.00 18.97
   ATOM  1975  CA  ASN A 255  0   17.583  10.479   9.599  1.00 17.69
   ATOM  1976  C   ASN A 255  0   16.785  10.335  10.889  1.00 17.64
10 ATOM  1977  O   ASN A 255  0   16.390   9.204  11.249  1.00 17.75
   ATOM  1978  CB  ASN A 255  0   16.663  10.554   8.386  1.00 17.19
   ATOM  1979  CG  ASN A 255  0   17.467  10.882   7.143  1.00 17.33
   ATOM  1980  OD1 ASN A 255  0   17.891  12.023   6.932  1.00 18.05
   ATOM  1981  ND2 ASN A 255  0   17.649   9.913   6.263  1.00 15.98
15 ATOM  1982  N   TYR A 256  0   16.657  11.403  11.684  1.00 14.89
   ATOM  1983  CA  TYR A 256  0   15.983  11.364  12.961  1.00 12.56
   ATOM  1984  C   TYR A 256  0   14.966  12.520  12.991  1.00 15.02
   ATOM  1985  O   TYR A 256  0   15.208  13.637  12.509  1.00 14.49
   ATOM  1986  CB  TYR A 256  0   16.867  11.479  14.216  1.00 14.85
20 ATOM  1987  CG  TYR A 256  0   17.883  10.349  14.316  1.00 13.96
   ATOM  1988  CD1 TYR A 256  0   19.030  10.427  13.529  1.00 13.97
   ATOM  1989  CD2 TYR A 256  0   17.712   9.245  15.129  1.00 14.62
   ATOM  1990  CE1 TYR A 256  0   19.986   9.422  13.534  1.00 13.83
   ATOM  1991  CE2 TYR A 256  0   18.667   8.224  15.170  1.00 15.31
25 ATOM  1992  CZ  TYR A 256  0   19.795   8.336  14.346  1.00 15.90
   ATOM  1993  OH  TYR A 256  0   20.763   7.341  14.337  1.00 17.15
   ATOM  1994  N   TRP A 257  0   13.801  12.198  13.564  1.00 13.58
   ATOM  1995  CA  TRP A 257  0   12.742  13.196  13.657  1.00 14.21
   ATOM  1996  C   TRP A 257  0   13.041  14.198  14.769  1.00 12.04
30 ATOM  1997  O   TRP A 257  0   13.382  13.811  15.878  1.00 10.46
   ATOM  1998  CB  TRP A 257  0   11.363  12.592  13.988  1.00 12.49
   ATOM  1999  CG  TRP A 257  0   10.648  11.906  12.865  1.00 13.06
   ATOM  2000  CD1 TRP A 257  0   10.315  10.568  12.879  1.00 12.86
   ATOM  2001  CD2 TRP A 257  0   10.161  12.437  11.633  1.00 12.33
35 ATOM  2002  NE1 TRP A 257  0    9.640  10.267  11.720  1.00 13.75
   ATOM  2003  CE2 TRP A 257  0    9.530  11.388  10.940  1.00 13.78
   ATOM  2004  CE3 TRP A 257  0   10.173  13.691  11.035  1.00 14.13
   ATOM  2005  CZ2 TRP A 257  0    8.940  11.538   9.681  1.00 13.24
```

```
      ATOM  2006  CZ3 TRP A 257  0   9.590 13.868  9.786 1.00 14.34
      ATOM  2007  CH2 TRP A 257  0   8.963 12.789  9.127 1.00 13.64
      ATOM  2008  N   ILE A 258  0  12.790 15.463 14.454 1.00 12.29
      ATOM  2009  CA  ILE A 258  0  12.886 16.498 15.508 1.00 12.44
   5  ATOM  2010  C   ILE A 258  0  11.391 16.840 15.769 1.00 12.40
      ATOM  2011  O   ILE A 258  0  10.629 17.039 14.812 1.00 12.43
      ATOM  2012  CB  ILE A 258  0  13.617 17.777 15.048 1.00 13.32
      ATOM  2013  CG1 ILE A 258  0  15.107 17.477 14.854 1.00 14.52
      ATOM  2014  CG2 ILE A 258  0  13.365 18.888 16.052 1.00 12.32
  10  ATOM  2015  CD1 ILE A 258  0  15.839 18.474 13.994 1.00 14.35
      ATOM  2016  N   ARG A 259  0  11.017 16.764 17.013 1.00 11.51
      ATOM  2017  CA  ARG A 259  0   9.610 16.832 17.407 1.00 13.43
      ATOM  2018  C   ARG A 259  0   9.254 18.019 18.274 1.00 12.74
      ATOM  2019  O   ARG A 259  0   9.931 18.246 19.280 1.00 12.62
  15  ATOM  2020  CB  ARG A 259  0   9.326 15.567 18.253 1.00 12.43
      ATOM  2021  CG  ARG A 259  0   9.308 14.290 17.414 1.00 15.81
      ATOM  2022  CD  ARG A 259  0   8.910 13.054 18.244 1.00 16.58
      ATOM  2023  NE  ARG A 259  0   9.204 11.818 17.528 1.00 16.91
      ATOM  2024  CZ  ARG A 259  0   8.475 11.187 16.616 1.00 18.43
  20  ATOM  2025  NH1 ARG A 259  0   7.285 11.657 16.239 1.00 19.39
      ATOM  2026  NH2 ARG A 259  0   8.907 10.070 16.045 1.00 17.95
      ATOM  2027  N   ALA A 260  0   8.226 18.764 17.884 1.00 13.12
      ATOM  2028  CA  ALA A 260  0   7.768 19.882 18.727 1.00 12.65
      ATOM  2029  C   ALA A 260  0   6.237 19.763 18.802 1.00 14.47
  25  ATOM  2030  O   ALA A 260  0   5.545 20.140 17.868 1.00 14.73
      ATOM  2031  CB  ALA A 260  0   8.281 21.188 18.165 1.00  9.58
      ATOM  2032  N   GLN A 261  0   5.690 19.225 19.870 1.00 14.78
      ATOM  2033  CA  GLN A 261  0   4.272 19.004 20.060 1.00 16.99
      ATOM  2034  C   GLN A 261  0   3.606 20.154 20.803 1.00 15.01
  30  ATOM  2035  O   GLN A 261  0   3.914 20.389 21.961 1.00 13.86
      ATOM  2036  CB  GLN A 261  0   4.118 17.747 20.924 1.00 20.94
      ATOM  2037  CG  GLN A 261  0   2.717 17.131 20.940 1.00 27.53
      ATOM  2038  CD  GLN A 261  0   2.721 15.991 21.947 1.00 29.63
      ATOM  2039  OE1 GLN A 261  0   3.152 14.887 21.682 1.00 31.60
  35  ATOM  2040  NE2 GLN A 261  0   2.331 16.255 23.188 1.00 34.91
      ATOM  2041  N   PRO A 262  0   2.663 20.820 20.167 1.00 14.60
      ATOM  2042  CA  PRO A 262  0   1.974 21.969 20.739 1.00 15.72
      ATOM  2043  C   PRO A 262  0   0.921 21.568 21.757 1.00 16.25
```

ATOM 2044 O PRO A 262 0 0.498 20.409 21.814 1.00 15.61
ATOM 2045 CB PRO A 262 0 1.401 22.752 19.539 1.00 13.88
ATOM 2046 CG PRO A 262 0 1.168 21.608 18.563 1.00 13.62
ATOM 2047 CD PRO A 262 0 2.257 20.570 18.772 1.00 13.23
5 ATOM 2048 N ASN A 263 0 0.570 22.481 22.665 1.00 17.25
ATOM 2049 CA ASN A 263 0 -0.471 22.203 23.648 1.00 17.50
ATOM 2050 C ASN A 263 0 -1.834 22.460 22.981 1.00 18.43
ATOM 2051 O ASN A 263 0 -2.810 22.121 23.608 1.00 19.35
ATOM 2052 CB ASN A 263 0 -0.422 22.990 24.954 1.00 16.12
10 ATOM 2053 CG ASN A 263 0 -0.333 24.493 24.728 1.00 16.97
ATOM 2054 OD1 ASN A 263 0 0.236 25.002 23.751 1.00 15.54
ATOM 2055 ND2 ASN A 263 0 -0.905 25.269 25.653 1.00 16.31
ATOM 2056 N LYS A 264 0 -1.947 23.055 21.818 1.00 20.51
ATOM 2057 CA LYS A 264 0 -3.256 23.208 21.180 1.00 24.76
15 ATOM 2058 C LYS A 264 0 -3.055 23.395 19.683 1.00 23.64
ATOM 2059 O LYS A 264 0 -1.909 23.572 19.267 1.00 24.23
ATOM 2060 CB LYS A 264 0 -4.038 24.393 21.775 1.00 25.87
ATOM 2061 CG LYS A 264 0 -3.266 25.702 21.602 1.00 28.62
ATOM 2062 CD LYS A 264 0 -3.579 26.624 22.772 1.00 30.65
20 ATOM 2063 CE LYS A 264 0 -4.114 27.960 22.283 1.00 32.62
ATOM 2064 NZ LYS A 264 0 -4.593 28.753 23.459 1.00 34.39
ATOM 2065 N GLY A 265 0 -4.112 23.386 18.892 1.00 22.60
ATOM 2066 CA GLY A 265 0 -3.959 23.591 17.452 1.00 22.98
ATOM 2067 C GLY A 265 0 -5.190 23.002 16.758 1.00 23.95
25 ATOM 2068 O GLY A 265 0 -5.904 22.202 17.362 1.00 22.64
ATOM 2069 N ARG A 266 0 -5.398 23.434 15.537 1.00 24.60
ATOM 2070 CA ARG A 266 0 -6.527 23.051 14.734 1.00 26.24
ATOM 2071 C ARG A 266 0 -6.412 21.605 14.272 1.00 27.29
ATOM 2072 O ARG A 266 0 -5.329 21.074 14.015 1.00 25.41
30 ATOM 2073 CB ARG A 266 0 -6.628 23.903 13.469 1.00 30.71
ATOM 2074 CG ARG A 266 0 -7.065 25.334 13.563 1.00 35.66
ATOM 2075 CD ARG A 266 0 -8.161 25.673 12.539 1.00 40.48
ATOM 2076 NE ARG A 266 0 -9.379 25.957 13.286 1.00 45.08
ATOM 2077 CZ ARG A 266 0 -10.551 25.334 13.319 1.00 47.09
35 ATOM 2078 NH1 ARG A 266 0 -10.921 24.294 12.577 1.00 48.10
ATOM 2079 NH2 ARG A 266 0 -11.452 25.828 14.165 1.00 47.80
ATOM 2080 N ASN A 267 0 -7.586 20.983 14.141 1.00 25.17
ATOM 2081 CA ASN A 267 0 -7.727 19.669 13.602 1.00 23.96

```
    ATOM  2082 C   ASN A 267 0  -6.859 18.625 14.244 1.00 22.35
    ATOM  2083 O   ASN A 267 0  -6.306 17.864 13.448 1.00 23.57
    ATOM  2084 CB  ASN A 267 0  -7.390 19.695 12.098 1.00 26.46
    ATOM  2085 CG  ASN A 267 0  -8.461 20.426 11.309 1.00 29.21
 5  ATOM  2086 OD1 ASN A 267 0  -8.190 21.226 10.405 1.00 30.18
    ATOM  2087 ND2 ASN A 267 0  -9.681 20.075 11.701 1.00 28.77
    ATOM  2088 N   GLY A 268 0  -6.706 18.594 15.550 1.00 21.85
    ATOM  2089 CA  GLY A 268 0  -5.890 17.533 16.121 1.00 22.47
    ATOM  2090 C   GLY A 268 0  -4.383 17.760 16.118 1.00 23.29
10  ATOM  2091 O   GLY A 268 0  -3.652 16.898 16.632 1.00 23.28
    ATOM  2092 N   LEU A 269 0  -3.880 18.901 15.676 1.00 22.69
    ATOM  2093 CA  LEU A 269 0  -2.454 19.222 15.684 1.00 22.62
    ATOM  2094 C   LEU A 269 0  -1.753 18.890 16.990 1.00 23.26
    ATOM  2095 O   LEU A 269 0  -0.650 18.335 17.035 1.00 23.42
15  ATOM  2096 CB  LEU A 269 0  -2.311 20.713 15.472 1.00 22.28
    ATOM  2097 CG  LEU A 269 0  -1.183 21.414 14.745 1.00 23.42
    ATOM  2098 CD1 LEU A 269 0  -0.508 22.380 15.682 1.00 19.64
    ATOM  2099 CD2 LEU A 269 0  -0.213 20.492 14.009 1.00 21.26
    ATOM  2100 N   ALA A 270 0  -2.371 19.199 18.135 1.00 21.51
20  ATOM  2101 CA  ALA A 270 0  -1.784 18.899 19.419 1.00 22.26
    ATOM  2102 C   ALA A 270 0  -1.612 17.415 19.680 1.00 23.22
    ATOM  2103 O   ALA A 270 0  -0.898 17.077 20.637 1.00 21.81
    ATOM  2104 CB  ALA A 270 0  -2.632 19.518 20.542 1.00 21.06
    ATOM  2105 N   GLY A 271 0  -2.337 16.521 18.996 1.00 23.75
25  ATOM  2106 CA  GLY A 271 0  -2.190 15.125 19.372 1.00 24.98
    ATOM  2107 C   GLY A 271 0  -1.507 14.267 18.328 1.00 26.07
    ATOM  2108 O   GLY A 271 0  -1.501 13.045 18.523 1.00 26.26
    ATOM  2109 N   THR A 272 0  -0.906 14.825 17.278 1.00 26.48
    ATOM  2110 CA  THR A 272 0  -0.327 13.901 16.294 1.00 25.27
30  ATOM  2111 C   THR A 272 0   0.986 14.362 15.701 1.00 25.58
    ATOM  2112 O   THR A 272 0   1.216 15.567 15.701 1.00 24.46
    ATOM  2113 CB  THR A 272 0  -1.380 13.759 15.164 1.00 24.40
    ATOM  2114 OG1 THR A 272 0  -0.931 12.737 14.275 1.00 26.32
    ATOM  2115 CG2 THR A 272 0  -1.575 15.022 14.347 1.00 22.50
35  ATOM  2116 N   PHE A 273 0   1.714 13.443 15.062 1.00 24.01
    ATOM  2117 CA  PHE A 273 0   2.897 13.755 14.271 1.00 23.99
    ATOM  2118 C   PHE A 273 0   2.663 13.201 12.858 1.00 24.84
    ATOM  2119 O   PHE A 273 0   3.534 13.207 11.987 1.00 24.73
```

```
    ATOM  2120 CB  PHE A 273  0   4.175 13.094 14.812 1.00 22.16
    ATOM  2121 CG  PHE A 273  0   4.550 13.676 16.153 1.00 21.84
    ATOM  2122 CD1 PHE A 273  0   4.190 13.037 17.327 1.00 20.67
    ATOM  2123 CD2 PHE A 273  0   5.221 14.881 16.216 1.00 20.98
  5 ATOM  2124 CE1 PHE A 273  0   4.538 13.574 18.554 1.00 21.75
    ATOM  2125 CE2 PHE A 273  0   5.559 15.428 17.440 1.00 21.65
    ATOM  2126 CZ  PHE A 273  0   5.216 14.787 18.616 1.00 22.38
    ATOM  2127 N   ALA A 274  0   1.440 12.718 12.647 1.00 24.38
    ATOM  2128 CA  ALA A 274  0   1.094 12.053 11.397 1.00 24.29
 10 ATOM  2129 C   ALA A 274  0   1.399 12.920 10.194 1.00 24.15
    ATOM  2130 O   ALA A 274  0   0.990 14.078 10.161 1.00 23.07
    ATOM  2131 CB  ALA A 274  0  -0.385 11.681 11.387 1.00 23.53
    ATOM  2132 N   ASN A 275  0   2.075 12.355  9.204 1.00 23.41
    ATOM  2133 CA  ASN A 275  0   2.389 13.068  7.987 1.00 24.88
 15 ATOM  2134 C   ASN A 275  0   3.498 14.093  8.191 1.00 22.73
    ATOM  2135 O   ASN A 275  0   3.708 14.947  7.337 1.00 21.57
    ATOM  2136 CB  ASN A 275  0   1.138 13.806  7.516 1.00 30.04
    ATOM  2137 CG  ASN A 275  0   0.194 13.070  6.633 1.00 35.28
    ATOM  2138 OD1 ASN A 275  0  -0.458 12.071  6.985 1.00 36.92
 20 ATOM  2139 ND2 ASN A 275  0   0.156 13.655  5.427 1.00 37.87
    ATOM  2140 N   GLY A 276  0   4.185 14.083  9.322 1.00 22.10
    ATOM  2141 CA  GLY A 276  0   5.278 15.025  9.503 1.00 20.95
    ATOM  2142 C   GLY A 276  0   4.801 16.392  9.962 1.00 19.61
    ATOM  2143 O   GLY A 276  0   5.587 17.325  9.816 1.00 19.96
 25 ATOM  2144 N   VAL A 277  0   3.600 16.504 10.540 1.00 16.82
    ATOM  2145 CA  VAL A 277  0   3.207 17.796 11.107 1.00 15.06
    ATOM  2146 C   VAL A 277  0   4.033 17.942 12.379 1.00 13.80
    ATOM  2147 O   VAL A 277  0   4.454 16.912 12.926 1.00 13.80
    ATOM  2148 CB  VAL A 277  0   1.676 17.849 11.397 1.00 14.37
 30 ATOM  2149 CG1 VAL A 277  0   0.882 17.824 10.099 1.00 13.37
    ATOM  2150 CG2 VAL A 277  0   1.213 16.763 12.330 1.00 11.77
    ATOM  2151 N   ASN A 278  0   4.307 19.100 12.936 1.00 14.25
    ATOM  2152 CA  ASN A 278  0   5.026 19.262 14.209 1.00 13.80
    ATOM  2153 C   ASN A 278  0   6.443 18.640 14.208 1.00 13.80
 35 ATOM  2154 O   ASN A 278  0   7.020 18.228 15.229 1.00 11.81
    ATOM  2155 CB  ASN A 278  0   4.216 18.607 15.312 1.00 14.24
    ATOM  2156 CG  ASN A 278  0   2.890 19.288 15.659 1.00 15.35
    ATOM  2157 OD1 ASN A 278  0   1.952 18.531 16.009 1.00 14.81
```

```
   ATOM   2158 ND2 ASN A 278  0   2.821 20.591 15.593 1.00 10.69
   ATOM   2159 N   SER A 279  0   7.044 18.595 13.025 1.00 12.68
   ATOM   2160 CA  SER A 279  0   8.296 17.892 12.860 1.00 15.48
   ATOM   2161 C   SER A 279  0   9.323 18.571 11.964 1.00 15.07
 5 ATOM   2162 O   SER A 279  0   8.995 19.309 11.044 1.00 12.20
   ATOM   2163 CB  SER A 279  0   7.976 16.549 12.122 1.00 14.76
   ATOM   2164 OG  SER A 279  0   7.268 15.722 13.054 1.00 19.57
   ATOM   2165 N   ALA A 280  0  10.570 18.152 12.229 1.00 15.67
   ATOM   2166 CA  ALA A 280  0  11.664 18.548 11.327 1.00 16.75
10 ATOM   2167 C   ALA A 280  0  12.620 17.341 11.287 1.00 15.83
   ATOM   2168 O   ALA A 280  0  12.438 16.346 11.997 1.00 15.55
   ATOM   2169 CB  ALA A 280  0  12.363 19.828 11.745 1.00 16.40
   ATOM   2170 N   ILE A 281  0  13.669 17.478 10.485 1.00 14.79
   ATOM   2171 CA  ILE A 281  0  14.569 16.346 10.257 1.00 15.55
15 ATOM   2172 C   ILE A 281  0  16.002 16.610 10.699 1.00 15.92
   ATOM   2173 O   ILE A 281  0  16.649 17.577 10.284 1.00 14.96
   ATOM   2174 CB  ILE A 281  0  14.557 16.013  8.735 1.00 16.44
   ATOM   2175 CG1 ILE A 281  0  13.147 15.573  8.275 1.00 16.42
   ATOM   2176 CG2 ILE A 281  0  15.615 14.959  8.421 1.00 15.71
20 ATOM   2177 CD1 ILE A 281  0  12.981 15.376  6.771 1.00 14.22
   ATOM   2178 N   LEU A 282  0  16.505 15.698 11.515 1.00 16.76
   ATOM   2179 CA  LEU A 282  0  17.920 15.736 11.912 1.00 15.82
   ATOM   2180 C   LEU A 282  0  18.655 14.747 10.990 1.00 16.16
   ATOM   2181 O   LEU A 282  0  18.409 13.530 11.034 1.00 16.41
25 ATOM   2182 CB  LEU A 282  0  18.129 15.400 13.379 1.00 14.54
   ATOM   2183 CG  LEU A 282  0  19.632 15.346 13.773 1.00 16.00
   ATOM   2184 CD1 LEU A 282  0  20.100 16.767 14.052 1.00 16.10
   ATOM   2185 CD2 LEU A 282  0  19.865 14.469 14.970 1.00 13.21
   ATOM   2186 N   ARG A 283  0  19.490 15.254 10.100 1.00 15.20
30 ATOM   2187 CA  ARG A 283  0  20.160 14.377  9.141 1.00 16.98
   ATOM   2188 C   ARG A 283  0  21.683 14.326  9.279 1.00 17.31
   ATOM   2189 O   ARG A 283  0  22.398 15.330  9.203 1.00 17.82
   ATOM   2190 CB  ARG A 283  0  19.844 14.861  7.736 1.00 17.30
   ATOM   2191 CG  ARG A 283  0  20.417 13.978  6.641 1.00 19.94
35 ATOM   2192 CD  ARG A 283  0  19.860 14.446  5.301 1.00 20.04
   ATOM   2193 NE  ARG A 283  0  18.474 14.010  5.208 1.00 21.56
   ATOM   2194 CZ  ARG A 283  0  17.479 14.530  4.505 1.00 21.81
   ATOM   2195 NH1 ARG A 283  0  16.287 13.922  4.564 1.00 21.52
```

88

```
    ATOM 2196 NH2 ARG A 283 0  17.653 15.634  3.797 1.00 21.84
    ATOM 2197 N   TYR A 284 0  22.163 13.136  9.567 1.00 16.79
    ATOM 2198 CA  TYR A 284 0  23.581 12.821  9.620 1.00 16.35
    ATOM 2199 C   TYR A 284 0  24.155 12.787  8.198 1.00 16.52
  5 ATOM 2200 O   TYR A 284 0  23.556 12.226  7.271 1.00 16.33
    ATOM 2201 CB  TYR A 284 0  23.730 11.444 10.252 1.00 16.51
    ATOM 2202 CG  TYR A 284 0  23.727 11.460 11.755 1.00 17.09
    ATOM 2203 CD1 TYR A 284 0  24.910 11.178 12.437 1.00 17.37
    ATOM 2204 CD2 TYR A 284 0  22.601 11.753 12.504 1.00 17.15
 10 ATOM 2205 CE1 TYR A 284 0  24.937 11.163 13.817 1.00 17.64
    ATOM 2206 CE2 TYR A 284 0  22.623 11.770 13.892 1.00 15.66
    ATOM 2207 CZ  TYR A 284 0  23.796 11.476 14.542 1.00 15.99
    ATOM 2208 OH  TYR A 284 0  23.873 11.448 15.919 1.00 14.03
    ATOM 2209 N   ALA A 285 0  25.276 13.463  7.992 1.00 17.42
 15 ATOM 2210 CA  ALA A 285 0  25.950 13.461  6.692 1.00 19.35
    ATOM 2211 C   ALA A 285 0  26.186 11.994  6.328 1.00 19.20
    ATOM 2212 O   ALA A 285 0  26.692 11.237  7.146 1.00 17.18
    ATOM 2213 CB  ALA A 285 0  27.293 14.194  6.770 1.00 19.86
    ATOM 2214 N   GLY A 286 0  25.724 11.614  5.153 1.00 20.01
 20 ATOM 2215 CA  GLY A 286 0  25.851 10.224  4.747 1.00 21.88
    ATOM 2216 C   GLY A 286 0  24.507  9.510  4.754 1.00 22.87
    ATOM 2217 O   GLY A 286 0  24.406  8.418  4.197 1.00 23.06
    ATOM 2218 N   ALA A 287 0  23.504 10.076  5.423 1.00 22.81
    ATOM 2219 CA  ALA A 287 0  22.176  9.449  5.364 1.00 21.50
 25 ATOM 2220 C   ALA A 287 0  21.482  9.880  4.079 1.00 20.58
    ATOM 2221 O   ALA A 287 0  21.647 11.032  3.629 1.00 19.44
    ATOM 2222 CB  ALA A 287 0  21.340  9.890  6.562 1.00 21.34
    ATOM 2223 N   ALA A 288 0  20.632  9.041  3.523 1.00 21.20
    ATOM 2224 CA  ALA A 288 0  19.899  9.450  2.310 1.00 23.46
 30 ATOM 2225 C   ALA A 288 0  18.965 10.629  2.513 1.00 24.70
    ATOM 2226 O   ALA A 288 0  18.494 10.929  3.621 1.00 25.30
    ATOM 2227 CB  ALA A 288 0  19.012  8.298  1.827 1.00 24.84
    ATOM 2228 N   ASN A 289 0  18.638 11.300  1.411 1.00 25.98
    ATOM 2229 CA  ASN A 289 0  17.674 12.398  1.439 1.00 27.16
 35 ATOM 2230 C   ASN A 289 0  16.303 11.707  1.505 1.00 27.36
    ATOM 2231 O   ASN A 289 0  15.761 11.330  0.477 1.00 27.56
    ATOM 2232 CB  ASN A 289 0  17.784 13.250  0.189 1.00 29.01
    ATOM 2233 CG  ASN A 289 0  18.808 14.364  0.299 1.00 30.44
```

```
    ATOM  2234 OD1 ASN A 289 0  20.005 14.168  0.545 1.00 30.40
    ATOM  2235 ND2 ASN A 289 0  18.340 15.591  0.121 1.00 31.98
    ATOM  2236 N   ALA A 290 0  15.837 11.426  2.703 1.00 25.22
    ATOM  2237 CA  ALA A 290 0  14.600 10.727  2.955 1.00 25.09
  5 ATOM  2238 C   ALA A 290 0  14.087 11.057  4.363 1.00 22.98
    ATOM  2239 O   ALA A 290 0  14.830 11.555  5.205 1.00 22.02
    ATOM  2240 CB  ALA A 290 0  14.764  9.210  2.823 1.00 24.89
    ATOM  2241 N   ASP A 291 0  12.822 10.718  4.597 1.00 21.88
    ATOM  2242 CA  ASP A 291 0  12.223 10.985  5.907 1.00 21.71
 10 ATOM  2243 C   ASP A 291 0  12.724  9.965  6.916 1.00 18.93
    ATOM  2244 O   ASP A 291 0  12.911  8.814  6.596 1.00 19.66
    ATOM  2245 CB  ASP A 291 0  10.695 10.862  5.834 1.00 22.63
    ATOM  2246 CG  ASP A 291 0  10.088 12.005  5.076 1.00 25.41
    ATOM  2247 OD1 ASP A 291 0  10.781 12.988  4.735 1.00 27.11
 15 ATOM  2248 OD2 ASP A 291 0   8.885 11.932  4.812 1.00 27.47
    ATOM  2249 N   PRO A 292 0  12.863 10.362  8.164 1.00 16.14
    ATOM  2250 CA  PRO A 292 0  13.229  9.473  9.230 1.00 15.27
    ATOM  2251 C   PRO A 292 0  12.087  8.484  9.389 1.00 19.40
    ATOM  2252 O   PRO A 292 0  10.925  8.785  9.063 1.00 20.36
 20 ATOM  2253 CB  PRO A 292 0  13.257 10.335 10.511 1.00 14.68
    ATOM  2254 CG  PRO A 292 0  13.291 11.739  9.941 1.00 14.39
    ATOM  2255 CD  PRO A 292 0  12.606 11.735  8.593 1.00 14.02
    ATOM  2256 N   THR A 293 0  12.357  7.361 10.024 1.00 19.91
    ATOM  2257 CA  THR A 293 0  11.360  6.379 10.373 1.00 20.62
 25 ATOM  2258 C   THR A 293 0  11.589  6.055 11.847 1.00 20.83
    ATOM  2259 O   THR A 293 0  11.323  4.943 12.287 1.00 23.91
    ATOM  2260 CB  THR A 293 0  11.556  5.088  9.557 1.00 23.41
    ATOM  2261 OG1 THR A 293 0  12.874  4.577  9.836 1.00 24.50
    ATOM  2262 CG2 THR A 293 0  11.438  5.341  8.058 1.00 23.72
 30 ATOM  2263 N   THR A 294 0  12.172  6.958 12.624 1.00 19.30
    ATOM  2264 CA  THR A 294 0  12.440  6.634 14.017 1.00 19.42
    ATOM  2265 C   THR A 294 0  11.214  6.896 14.878 1.00 20.66
    ATOM  2266 O   THR A 294 0  10.240  7.485 14.411 1.00 19.89
    ATOM  2267 CB  THR A 294 0  13.565  7.548 14.553 1.00 19.28
 35 ATOM  2268 OG1 THR A 294 0  13.174  8.889 14.251 1.00 17.55
    ATOM  2269 CG2 THR A 294 0  14.860  7.214 13.822 1.00 19.27
    ATOM  2270 N   SER A 295 0  11.359  6.576 16.159 1.00 23.85
    ATOM  2271 CA  SER A 295 0  10.274  6.851 17.095 1.00 27.18
```

ATOM 2272 C   SER A 295 0 10.781 7.484 18.375 1.00 27.92
ATOM 2273 O   SER A 295 0 11.900 7.292 18.844 1.00 27.09
ATOM 2274 CB SER A 295 0   9.513 5.546 17.367 1.00 28.92
ATOM 2275 OG SER A 295 0 10.389 4.761 18.160 1.00 33.04
5 ATOM 2276 N   ALA A 296 0   9.930 8.331 18.965 1.00 30.04
ATOM 2277 CA ALA A 296 0 10.295 9.003 20.207 1.00 29.82
ATOM 2278 C   ALA A 296 0 10.552 8.011 21.327 1.00 30.83
ATOM 2279 O   ALA A 296 0 10.114 6.861 21.328 1.00 30.67
ATOM 2280 CB ALA A 296 0   9.187 9.968 20.599 1.00 30.16
10 ATOM 2281 N   ASN A 297 0 11.286 8.489 22.328 1.00 31.65
ATOM 2282 CA ASN A 297 0 11.543 7.750 23.549 1.00 32.16
ATOM 2283 C   ASN A 297 0 10.200 7.650 24.285 1.00 32.80
ATOM 2284 O   ASN A 297 0   9.492 8.616 24.565 1.00 31.30
ATOM 2285 CB ASN A 297 0 12.522 8.497 24.443 1.00 33.07
15 ATOM 2286 CG ASN A 297 0 12.869 7.742 25.706 1.00 35.21
ATOM 2287 OD1 ASN A 297 0 12.116 6.965 26.284 1.00 35.45
ATOM 2288 ND2 ASN A 297 0 14.106 7.982 26.162 1.00 37.10
ATOM 2289 N   PRO A 298 0   9.865 6.430 24.647 1.00 33.40
ATOM 2290 CA PRO A 298 0   8.626 6.116 25.331 1.00 33.89
20 ATOM 2291 C   PRO A 298 0   8.580 6.690 26.732 1.00 32.60
ATOM 2292 O   PRO A 298 0   7.522 7.155 27.173 1.00 32.72
ATOM 2293 CB PRO A 298 0   8.505 4.576 25.358 1.00 35.13
ATOM 2294 CG PRO A 298 0   9.932 4.147 25.128 1.00 34.52
ATOM 2295 CD PRO A 298 0 10.630 5.222 24.323 1.00 34.10
25 ATOM 2296 N   ASN A 299 0   9.689 6.721 27.461 1.00 29.60
ATOM 2297 CA ASN A 299 0   9.701 7.229 28.834 1.00 28.47
ATOM 2298 C   ASN A 299 0 10.818 8.251 29.006 1.00 27.18
ATOM 2299 O   ASN A 299 0 11.906 7.967 29.528 1.00 25.69
ATOM 2300 CB ASN A 299 0   9.964 6.017 29.747 1.00 29.50
30 ATOM 2301 CG ASN A 299 0   8.907 4.935 29.673 1.00 32.34
ATOM 2302 OD1 ASN A 299 0   9.090 3.873 29.075 1.00 33.50
ATOM 2303 ND2 ASN A 299 0   7.735 5.182 30.251 1.00 33.04
ATOM 2304 N   PRO A 300 0 10.629 9.450 28.498 1.00 26.02
ATOM 2305 CA PRO A 300 0 11.668 10.486 28.498 1.00 23.99
35 ATOM 2306 C   PRO A 300 0 11.987 11.054 29.860 1.00 21.16
ATOM 2307 O   PRO A 300 0 11.051 11.174 30.649 1.00 20.81
ATOM 2308 CB PRO A 300 0 11.137 11.623 27.594 1.00 23.33
ATOM 2309 CG PRO A 300 0   9.645 11.422 27.729 1.00 24.68

ATOM 2310 CD PRO A 300 0 9.387 9.918 27.882 1.00 25.22
ATOM 2311 N ALA A 301 0 13.242 11.361 30.179 1.00 19.17
ATOM 2312 CA ALA A 301 0 13.538 12.139 31.410 1.00 17.57
ATOM 2313 C ALA A 301 0 13.159 13.588 31.084 1.00 16.53
5 ATOM 2314 O ALA A 301 0 13.613 14.235 30.131 1.00 16.24
ATOM 2315 CB ALA A 301 0 15.006 11.982 31.774 1.00 17.17
ATOM 2316 N GLN A 302 0 12.139 14.131 31.723 1.00 18.15
ATOM 2317 CA GLN A 302 0 11.580 15.446 31.441 1.00 19.34
ATOM 2318 C GLN A 302 0 12.335 16.580 32.124 1.00 19.16
10 ATOM 2319 O GLN A 302 0 12.577 16.444 33.324 1.00 19.07
ATOM 2320 CB GLN A 302 0 10.122 15.483 31.937 1.00 19.10
ATOM 2321 CG GLN A 302 0 9.304 16.666 31.478 1.00 20.55
ATOM 2322 CD GLN A 302 0 8.960 16.738 30.009 1.00 20.18
ATOM 2323 OE1 GLN A 302 0 8.843 15.721 29.331 1.00 22.29
15 ATOM 2324 NE2 GLN A 302 0 8.813 17.936 29.436 1.00 18.46
ATOM 2325 N LEU A 303 0 12.629 17.681 31.444 1.00 17.92
ATOM 2326 CA LEU A 303 0 13.241 18.824 32.139 1.00 17.32
ATOM 2327 C LEU A 303 0 12.316 19.357 33.232 1.00 17.65
ATOM 2328 O LEU A 303 0 11.140 19.664 33.021 1.00 17.55
20 ATOM 2329 CB LEU A 303 0 13.489 19.988 31.168 1.00 15.14
ATOM 2330 CG LEU A 303 0 13.919 21.317 31.797 1.00 16.94
ATOM 2331 CD1 LEU A 303 0 15.262 21.146 32.504 1.00 17.30
ATOM 2332 CD2 LEU A 303 0 13.988 22.432 30.764 1.00 12.82
ATOM 2333 N ASN A 304 0 12.868 19.580 34.399 1.00 17.34
25 ATOM 2334 CA ASN A 304 0 12.199 20.212 35.531 1.00 19.12
ATOM 2335 C ASN A 304 0 13.071 21.435 35.833 1.00 19.06
ATOM 2336 O ASN A 304 0 14.265 21.349 36.122 1.00 20.37
ATOM 2337 CB ASN A 304 0 12.073 19.244 36.704 1.00 22.16
ATOM 2338 CG ASN A 304 0 11.748 19.900 38.024 1.00 25.02
30 ATOM 2339 OD1 ASN A 304 0 11.506 21.111 38.146 1.00 26.72
ATOM 2340 ND2 ASN A 304 0 11.766 19.133 39.114 1.00 25.99
ATOM 2341 N GLU A 305 0 12.541 22.629 35.662 1.00 17.64
ATOM 2342 CA GLU A 305 0 13.204 23.890 35.840 1.00 16.64
ATOM 2343 C GLU A 305 0 13.884 23.977 37.194 1.00 16.06
35 ATOM 2344 O GLU A 305 0 14.965 24.564 37.208 1.00 14.78
ATOM 2345 CB GLU A 305 0 12.286 25.085 35.567 1.00 15.91
ATOM 2346 CG GLU A 305 0 12.898 26.484 35.831 1.00 14.81
ATOM 2347 CD GLU A 305 0 11.794 27.546 35.666 1.00 15.72

```
     ATOM   2348 OE1 GLU A 305 0  11.584 28.026 34.527 1.00 14.63
     ATOM   2349 OE2 GLU A 305 0  11.154 27.861 36.685 1.00 13.05
     ATOM   2350 N   ALA A 306 0  13.416 23.432 38.298 1.00 15.83
     ATOM   2351 CA  ALA A 306 0  14.131 23.509 39.565 1.00 17.92
  5  ATOM   2352 C   ALA A 306 0  15.437 22.682 39.532 1.00 18.62
     ATOM   2353 O   ALA A 306 0  16.213 22.867 40.464 1.00 18.37
     ATOM   2354 CB  ALA A 306 0  13.283 22.993 40.711 1.00 16.23
     ATOM   2355 N   ASP A 307 0  15.721 21.860 38.523 1.00 18.04
     ATOM   2356 CA  ASP A 307 0  16.988 21.164 38.409 1.00 18.68
 10  ATOM   2357 C   ASP A 307 0  18.035 22.039 37.707 1.00 19.89
     ATOM   2358 O   ASP A 307 0  19.239 21.695 37.739 1.00 20.36
     ATOM   2359 CB  ASP A 307 0  16.904 19.863 37.592 1.00 17.64
     ATOM   2360 CG  ASP A 307 0  15.980 18.873 38.290 1.00 18.17
     ATOM   2361 OD1 ASP A 307 0  15.918 18.919 39.535 1.00 18.27
 15  ATOM   2362 OD2 ASP A 307 0  15.311 18.094 37.592 1.00 17.32
     ATOM   2363 N   LEU A 308 0  17.583 23.110 37.052 1.00 16.43
     ATOM   2364 CA  LEU A 308 0  18.581 23.962 36.377 1.00 16.80
     ATOM   2365 C   LEU A 308 0  19.327 24.827 37.384 1.00 16.94
     ATOM   2366 O   LEU A 308 0  18.784 25.320 38.380 1.00 17.28
 20  ATOM   2367 CB  LEU A 308 0  17.925 24.775 35.257 1.00 12.52
     ATOM   2368 CG  LEU A 308 0  17.436 23.936 34.073 1.00 12.15
     ATOM   2369 CD1 LEU A 308 0  16.692 24.834 33.101 1.00 11.67
     ATOM   2370 CD2 LEU A 308 0  18.547 23.186 33.341 1.00 12.23
     ATOM   2371 N   HIS A 309 0  20.640 24.968 37.243 1.00 18.01
 25  ATOM   2372 CA  HIS A 309 0  21.430 25.802 38.158 1.00 18.47
     ATOM   2373 C   HIS A 309 0  22.328 26.770 37.394 1.00 17.36
     ATOM   2374 O   HIS A 309 0  23.015 26.378 36.459 1.00 17.82
     ATOM   2375 CB  HIS A 309 0  22.267 24.997 39.140 1.00 18.51
     ATOM   2376 CG  HIS A 309 0  21.470 24.052 39.965 1.00 20.71
 30  ATOM   2377 ND1 HIS A 309 0  21.526 22.684 39.790 1.00 21.77
     ATOM   2378 CD2 HIS A 309 0  20.578 24.285 40.956 1.00 22.07
     ATOM   2379 CE1 HIS A 309 0  20.701 22.115 40.657 1.00 22.85
     ATOM   2380 NE2 HIS A 309 0  20.120 23.059 41.377 1.00 22.67
     ATOM   2381 N   ALA A 310 0  22.352 28.005 37.837 1.00 17.27
 35  ATOM   2382 CA  ALA A 310 0  23.173 29.068 37.228 1.00 17.74
     ATOM   2383 C   ALA A 310 0  24.663 28.775 37.342 1.00 18.13
     ATOM   2384 O   ALA A 310 0  25.103 28.233 38.369 1.00 19.61
     ATOM   2385 CB  ALA A 310 0  22.869 30.356 37.985 1.00 16.92
```

```
    ATOM   2386  N   LEU A 311  0   25.427 29.021 36.304 1.00 19.30
    ATOM   2387  CA  LEU A 311  0   26.856 28.762 36.277 1.00 20.71
    ATOM   2388  C   LEU A 311  0   27.655 29.922 36.881 1.00 22.67
    ATOM   2389  O   LEU A 311  0   28.581 29.788 37.682 1.00 23.06
 5  ATOM   2390  CB  LEU A 311  0   27.305 28.591 34.817 1.00 20.57
    ATOM   2391  CG  LEU A 311  0   28.796 28.196 34.684 1.00 21.52
    ATOM   2392  CD1 LEU A 311  0   28.993 26.783 35.229 1.00 20.80
    ATOM   2393  CD2 LEU A 311  0   29.319 28.282 33.254 1.00 20.17
    ATOM   2394  N   ILE A 312  0   27.333 31.142 36.449 1.00 23.42
10  ATOM   2395  CA  ILE A 312  0   28.092 32.311 36.899 1.00 24.86
    ATOM   2396  C   ILE A 312  0   27.337 33.157 37.914 1.00 26.54
    ATOM   2397  O   ILE A 312  0   26.154 33.467 37.739 1.00 25.31
    ATOM   2398  CB  ILE A 312  0   28.397 33.179 35.670 1.00 24.45
    ATOM   2399  CG1 ILE A 312  0   28.998 32.330 34.576 1.00 25.60
15  ATOM   2400  CG2 ILE A 312  0   29.261 34.373 36.075 1.00 26.44
    ATOM   2401  CD1 ILE A 312  0   30.462 32.026 34.512 1.00 24.51
    ATOM   2402  N   ASP A 313  0   28.008 33.523 39.003 1.00 28.70
    ATOM   2403  CA  ASP A 313  0   27.432 34.339 40.071 1.00 30.99
    ATOM   2404  C   ASP A 313  0   26.065 33.763 40.417 1.00 29.83
20  ATOM   2405  O   ASP A 313  0   25.024 34.385 40.235 1.00 28.51
    ATOM   2406  CB  ASP A 313  0   27.266 35.777 39.576 1.00 35.88
    ATOM   2407  CG  ASP A 313  0   28.532 36.505 39.187 1.00 40.21
    ATOM   2408  OD1 ASP A 313  0   29.577 36.243 39.847 1.00 42.99
    ATOM   2409  OD2 ASP A 313  0   28.525 37.346 38.252 1.00 40.95
25  ATOM   2410  N   PRO A 314  0   26.041 32.517 40.863 1.00 28.77
    ATOM   2411  CA  PRO A 314  0   24.841 31.743 41.074 1.00 27.80
    ATOM   2412  C   PRO A 314  0   23.865 32.198 42.137 1.00 26.49
    ATOM   2413  O   PRO A 314  0   22.671 31.857 42.032 1.00 27.17
    ATOM   2414  CB  PRO A 314  0   25.297 30.311 41.479 1.00 27.61
30  ATOM   2415  CG  PRO A 314  0   26.711 30.573 41.929 1.00 29.37
    ATOM   2416  CD  PRO A 314  0   27.248 31.726 41.111 1.00 28.10
    ATOM   2417  N   ALA A 315  0   24.364 32.818 43.206 1.00 23.45
    ATOM   2418  CA  ALA A 315  0   23.505 33.092 44.336 1.00 22.34
    ATOM   2419  C   ALA A 315  0   22.414 34.111 44.008 1.00 22.46
35  ATOM   2420  O   ALA A 315  0   22.678 35.127 43.370 1.00 22.52
    ATOM   2421  CB  ALA A 315  0   24.294 33.617 45.532 1.00 21.68
    ATOM   2422  N   ALA A 316  0   21.226 33.838 44.534 1.00 20.85
    ATOM   2423  CA  ALA A 316  0   20.133 34.805 44.422 1.00 20.78
```

```
   ATOM 2424 C   ALA A 316 0  20.547 36.010 45.271 1.00 20.55
   ATOM 2425 O   ALA A 316 0  21.143 35.846 46.333 1.00 21.47
   ATOM 2426 CB  ALA A 316 0  18.897 34.166 45.043 1.00 18.32
   ATOM 2427 N   PRO A 317 0  20.237 37.212 44.864 1.00 20.84
 5 ATOM 2428 CA  PRO A 317 0  20.539 38.410 45.634 1.00 20.82
   ATOM 2429 C   PRO A 317 0  19.766 38.449 46.945 1.00 20.96
   ATOM 2430 O   PRO A 317 0  18.668 37.885 47.030 1.00 21.42
   ATOM 2431 CB  PRO A 317 0  20.064 39.590 44.758 1.00 21.64
   ATOM 2432 CG  PRO A 317 0  19.178 38.938 43.746 1.00 21.69
10 ATOM 2433 CD  PRO A 317 0  19.517 37.466 43.619 1.00 20.10
   ATOM 2434 N   GLY A 318 0  20.269 39.080 47.988 1.00 20.69
   ATOM 2435 CA  GLY A 318 0  19.533 39.282 49.225 1.00 21.68
   ATOM 2436 C   GLY A 318 0  19.631 38.218 50.283 1.00 22.93
   ATOM 2437 O   GLY A 318 0  20.344 37.221 50.101 1.00 23.87
15 ATOM 2438 N   ILE A 319 0  18.895 38.398 51.368 1.00 22.20
   ATOM 2439 CA  ILE A 319 0  18.879 37.432 52.454 1.00 24.16
   ATOM 2440 C   ILE A 319 0  18.169 36.189 51.956 1.00 25.28
   ATOM 2441 O   ILE A 319 0  17.071 36.271 51.405 1.00 26.26
   ATOM 2442 CB  ILE A 319 0  18.208 38.030 53.704 1.00 24.54
20 ATOM 2443 CG1 ILE A 319 0  19.075 39.176 54.213 1.00 25.08
   ATOM 2444 CG2 ILE A 319 0  17.944 37.012 54.793 1.00 24.03
   ATOM 2445 CD1 ILE A 319 0  18.262 40.183 55.006 1.00 27.56
   ATOM 2446 N   PRO A 320 0  18.762 35.030 52.159 1.00 26.23
   ATOM 2447 CA  PRO A 320 0  18.273 33.748 51.684 1.00 26.64
25 ATOM 2448 C   PRO A 320 0  17.105 33.172 52.453 1.00 26.74
   ATOM 2449 O   PRO A 320 0  17.140 32.025 52.896 1.00 27.54
   ATOM 2450 CB  PRO A 320 0  19.501 32.801 51.772 1.00 27.16
   ATOM 2451 CG  PRO A 320 0  20.216 33.388 52.985 1.00 25.20
   ATOM 2452 CD  PRO A 320 0  20.061 34.891 52.837 1.00 25.62
30 ATOM 2453 N   THR A 321 0  16.022 33.909 52.611 1.00 27.35
   ATOM 2454 CA  THR A 321 0  14.820 33.550 53.329 1.00 28.07
   ATOM 2455 C   THR A 321 0  13.632 34.190 52.603 1.00 27.48
   ATOM 2456 O   THR A 321 0  13.597 35.383 52.302 1.00 27.13
   ATOM 2457 CB  THR A 321 0  14.824 34.085 54.780 1.00 29.87
35 ATOM 2458 OG1 THR A 321 0  15.957 33.582 55.511 1.00 31.85
   ATOM 2459 CG2 THR A 321 0  13.548 33.687 55.507 1.00 31.06
   ATOM 2460 N   PRO A 322 0  12.630 33.378 52.326 1.00 26.63
   ATOM 2461 CA  PRO A 322 0  11.428 33.824 51.637 1.00 25.91
```

```
     ATOM   2462  C   PRO A 322  0   10.892 35.072 52.313 1.00 25.37
     ATOM   2463  O   PRO A 322  0   10.945 35.194 53.542 1.00 25.02
     ATOM   2464  CB  PRO A 322  0   10.456 32.638 51.661 1.00 26.11
     ATOM   2465  CG  PRO A 322  0   11.370 31.477 51.931 1.00 26.67
 5   ATOM   2466  CD  PRO A 322  0   12.592 31.961 52.691 1.00 26.21
     ATOM   2467  N   GLY A 323  0   10.432 36.075 51.573 1.00 24.30
     ATOM   2468  CA  GLY A 323  0    9.943 37.288 52.197 1.00 24.13
     ATOM   2469  C   GLY A 323  0   11.013 38.161 52.842 1.00 25.48
     ATOM   2470  O   GLY A 323  0   10.603 39.128 53.512 1.00 25.28
10   ATOM   2471  N   ALA A 324  0   12.320 37.959 52.688 1.00 24.80
     ATOM   2472  CA  ALA A 324  0   13.278 38.831 53.377 1.00 24.61
     ATOM   2473  C   ALA A 324  0   14.034 39.773 52.451 1.00 23.92
     ATOM   2474  O   ALA A 324  0   15.148 40.225 52.748 1.00 24.53
     ATOM   2475  CB  ALA A 324  0   14.255 38.012 54.204 1.00 23.79
15   ATOM   2476  N   ALA A 325  0   13.423 40.081 51.315 1.00 22.22
     ATOM   2477  CA  ALA A 325  0   14.033 40.985 50.341 1.00 20.42
     ATOM   2478  C   ALA A 325  0   13.825 42.423 50.803 1.00 19.97
     ATOM   2479  O   ALA A 325  0   12.987 42.648 51.677 1.00 18.14
     ATOM   2480  CB  ALA A 325  0   13.272 40.763 49.018 1.00 19.40
20   ATOM   2481  N   ASP A 326  0   14.422 43.421 50.161 1.00 20.69
     ATOM   2482  CA  ASP A 326  0   14.141 44.804 50.529 1.00 22.54
     ATOM   2483  C   ASP A 326  0   12.702 45.158 50.220 1.00 22.83
     ATOM   2484  O   ASP A 326  0   12.015 45.754 51.030 1.00 23.68
     ATOM   2485  CB  ASP A 326  0   15.089 45.767 49.789 1.00 22.32
25   ATOM   2486  CG  ASP A 326  0   16.494 45.378 50.238 1.00 23.83
     ATOM   2487  OD1 ASP A 326  0   16.650 45.284 51.475 1.00 24.78
     ATOM   2488  OD2 ASP A 326  0   17.393 45.171 49.409 1.00 24.90
     ATOM   2489  N   VAL A 327  0   12.254 44.821 49.026 1.00 24.29
     ATOM   2490  CA  VAL A 327  0   10.914 45.064 48.503 1.00 23.57
30   ATOM   2491  C   VAL A 327  0   10.246 43.721 48.170 1.00 23.46
     ATOM   2492  O   VAL A 327  0   10.785 42.933 47.386 1.00 22.62
     ATOM   2493  CB  VAL A 327  0   10.946 45.898 47.220 1.00 24.70
     ATOM   2494  CG1 VAL A 327  0    9.554 46.274 46.751 1.00 24.11
     ATOM   2495  CG2 VAL A 327  0   11.773 47.173 47.420 1.00 26.30
35   ATOM   2496  N   ASN A 328  0    9.113 43.463 48.811 1.00 21.44
     ATOM   2497  CA  ASN A 328  0    8.390 42.212 48.717 1.00 23.21
     ATOM   2498  C   ASN A 328  0    6.986 42.410 48.158 1.00 23.12
     ATOM   2499  O   ASN A 328  0    6.140 43.030 48.799 1.00 22.76
```

```
   ATOM  2500 CB  ASN A 328 0    8.223 41.603 50.121 1.00 23.09
   ATOM  2501 CG  ASN A 328 0    9.569 41.204 50.693 1.00 24.61
   ATOM  2502 OD1 ASN A 328 0   10.181 40.188 50.295 1.00 25.87
   ATOM  2503 ND2 ASN A 328 0   10.017 42.029 51.617 1.00 21.47
 5 ATOM  2504 N   LEU A 329 0    6.776 42.000 46.923 1.00 23.14
   ATOM  2505 CA  LEU A 329 0    5.497 42.179 46.268 1.00 24.23
   ATOM  2506 C   LEU A 329 0    4.859 40.822 45.953 1.00 25.21
   ATOM  2507 O   LEU A 329 0    5.489 39.876 45.469 1.00 24.20
   ATOM  2508 CB  LEU A 329 0    5.622 42.963 44.948 1.00 24.33
10 ATOM  2509 CG  LEU A 329 0    6.369 44.279 45.082 1.00 26.30
   ATOM  2510 CD1 LEU A 329 0    6.778 44.884 43.757 1.00 26.24
   ATOM  2511 CD2 LEU A 329 0    5.550 45.249 45.913 1.00 27.07
   ATOM  2512 N   ARG A 330 0    3.562 40.806 46.204 1.00 25.13
   ATOM  2513 CA  ARG A 330 0    2.740 39.641 45.899 1.00 27.48
15 ATOM  2514 C   ARG A 330 0    1.628 40.116 44.965 1.00 27.52
   ATOM  2515 O   ARG A 330 0    0.988 41.132 45.257 1.00 27.17
   ATOM  2516 CB  ARG A 330 0    2.200 39.017 47.166 1.00 29.82
   ATOM  2517 CG  ARG A 330 0    1.351 37.794 46.932 1.00 33.18
   ATOM  2518 CD  ARG A 330 0    0.880 37.251 48.284 1.00 37.06
20 ATOM  2519 NE  ARG A 330 0    0.305 35.914 48.038 1.00 40.34
   ATOM  2520 CZ  ARG A 330 0    1.009 34.803 48.298 1.00 40.82
   ATOM  2521 NH1 ARG A 330 0    2.229 34.903 48.812 1.00 40.36
   ATOM  2522 NH2 ARG A 330 0    0.415 33.642 48.040 1.00 41.33
   ATOM  2523 N   PHE A 331 0    1.507 39.481 43.795 1.00 25.88
25 ATOM  2524 CA  PHE A 331 0    0.475 39.937 42.855 1.00 25.87
   ATOM  2525 C   PHE A 331 0   -0.657 38.919 42.779 1.00 25.94
   ATOM  2526 O   PHE A 331 0   -0.441 37.697 42.824 1.00 24.61
   ATOM  2527 CB  PHE A 331 0    1.102 40.269 41.511 1.00 25.94
   ATOM  2528 CG  PHE A 331 0    1.884 41.565 41.496 1.00 28.66
30 ATOM  2529 CD1 PHE A 331 0    1.282 42.782 41.759 1.00 28.04
   ATOM  2530 CD2 PHE A 331 0    3.246 41.569 41.214 1.00 29.71
   ATOM  2531 CE1 PHE A 331 0    1.988 43.963 41.744 1.00 29.21
   ATOM  2532 CE2 PHE A 331 0    3.975 42.753 41.181 1.00 30.61
   ATOM  2533 CZ  PHE A 331 0    3.348 43.965 41.453 1.00 30.66
35 ATOM  2534 N   GLN A 332 0   -1.873 39.446 42.676 1.00 25.58
   ATOM  2535 CA  GLN A 332 0   -3.085 38.628 42.608 1.00 26.60
   ATOM  2536 C   GLN A 332 0   -3.672 38.698 41.203 1.00 23.61
   ATOM  2537 O   GLN A 332 0   -4.136 39.739 40.755 1.00 21.73
```

```
   ATOM 2538 CB  GLN A 332 0  -4.110 39.094 43.630 1.00 30.32
   ATOM 2539 CG  GLN A 332 0  -5.412 38.299 43.642 1.00 35.72
   ATOM 2540 CD  GLN A 332 0  -5.199 36.961 44.325 1.00 39.98
   ATOM 2541 OE1 GLN A 332 0  -5.859 35.961 44.007 1.00 42.32
 5 ATOM 2542 NE2 GLN A 332 0  -4.257 36.915 45.270 1.00 42.27
   ATOM 2543 N   LEU A 333 0  -3.612 37.576 40.504 1.00 23.60
   ATOM 2544 CA  LEU A 333 0  -4.105 37.565 39.118 1.00 26.25
   ATOM 2545 C   LEU A 333 0  -5.627 37.373 39.123 1.00 26.55
   ATOM 2546 O   LEU A 333 0  -6.107 36.655 39.998 1.00 25.70
10 ATOM 2547 CB  LEU A 333 0  -3.424 36.465 38.304 1.00 25.25
   ATOM 2548 CG  LEU A 333 0  -1.919 36.608 38.052 1.00 25.72
   ATOM 2549 CD1 LEU A 333 0  -1.431 35.565 37.067 1.00 23.66
   ATOM 2550 CD2 LEU A 333 0  -1.551 38.000 37.558 1.00 25.25
   ATOM 2551 N   GLY A 334 0  -6.327 37.976 38.188 1.00 27.85
15 ATOM 2552 CA  GLY A 334 0  -7.770 37.782 38.118 1.00 29.96
   ATOM 2553 C   GLY A 334 0  -8.253 37.802 36.672 1.00 32.36
   ATOM 2554 O   GLY A 334 0  -7.559 38.175 35.719 1.00 30.74
   ATOM 2555 N   PHE A 335 0  -9.502 37.377 36.544 1.00 34.76
   ATOM 2556 CA  PHE A 335 0 -10.181 37.360 35.260 1.00 38.54
20 ATOM 2557 C   PHE A 335 0 -11.625 37.806 35.514 1.00 41.05
   ATOM 2558 O   PHE A 335 0 -12.443 37.028 36.021 1.00 41.53
   ATOM 2559 CB  PHE A 335 0 -10.183 36.003 34.586 1.00 39.00
   ATOM 2560 CG  PHE A 335 0 -10.772 36.105 33.197 1.00 40.61
   ATOM 2561 CD1 PHE A 335 0 -10.052 36.686 32.175 1.00 40.45
25 ATOM 2562 CD2 PHE A 335 0 -12.045 35.614 32.942 1.00 41.39
   ATOM 2563 CE1 PHE A 335 0 -10.580 36.778 30.901 1.00 40.81
   ATOM 2564 CE2 PHE A 335 0 -12.588 35.697 31.671 1.00 41.51
   ATOM 2565 CZ  PHE A 335 0 -11.849 36.281 30.652 1.00 41.87
   ATOM 2566 N   SER A 336 0 -11.861 39.075 35.193 1.00 42.39
30 ATOM 2567 CA  SER A 336 0 -13.203 39.582 35.445 1.00 44.12
   ATOM 2568 C   SER A 336 0 -13.704 40.525 34.370 1.00 44.31
   ATOM 2569 O   SER A 336 0 -13.028 41.440 33.903 1.00 44.49
   ATOM 2570 CB  SER A 336 0 -13.214 40.206 36.842 1.00 45.46
   ATOM 2571 OG  SER A 336 0 -13.727 39.233 37.758 1.00 47.11
35 ATOM 2572 N   GLY A 337 0 -14.963 40.267 33.983 1.00 44.12
   ATOM 2573 CA  GLY A 337 0 -15.630 41.067 32.959 1.00 41.89
   ATOM 2574 C   GLY A 337 0 -14.963 40.920 31.608 1.00 40.08
   ATOM 2575 O   GLY A 337 0 -14.712 41.891 30.888 1.00 41.35
```

```
    ATOM   2576 N   GLY A 338  0  -14.583  39.699  31.263  1.00 39.12
    ATOM   2577 CA  GLY A 338  0  -13.899  39.364  30.034  1.00 36.11
    ATOM   2578 C   GLY A 338  0  -12.503  39.970  29.929  1.00 34.97
    ATOM   2579 O   GLY A 338  0  -12.005  40.116  28.806  1.00 33.64
 5  ATOM   2580 N   ARG A 339  0  -11.885  40.355  31.048  1.00 33.21
    ATOM   2581 CA  ARG A 339  0  -10.538  40.916  30.982  1.00 32.04
    ATOM   2582 C   ARG A 339  0   -9.724  40.397  32.164  1.00 29.23
    ATOM   2583 O   ARG A 339  0  -10.260  40.053  33.210  1.00 26.38
    ATOM   2584 CB  ARG A 339  0  -10.495  42.419  30.845  1.00 36.52
10  ATOM   2585 CG  ARG A 339  0  -11.291  43.281  31.790  1.00 42.08
    ATOM   2586 CD  ARG A 339  0  -11.895  44.502  31.127  1.00 45.03
    ATOM   2587 NE  ARG A 339  0  -11.046  45.380  30.351  1.00 47.77
    ATOM   2588 CZ  ARG A 339  0  -10.635  46.616  30.664  1.00 49.55
    ATOM   2589 NH1 ARG A 339  0  -10.935  47.242  31.799  1.00 49.60
15  ATOM   2590 NH2 ARG A 339  0   -9.862  47.295  29.805  1.00 49.96
    ATOM   2591 N   PHE A 340  0   -8.425  40.181  31.900  1.00 25.50
    ATOM   2592 CA  PHE A 340  0   -7.526  39.713  32.938  1.00 22.68
    ATOM   2593 C   PHE A 340  0   -7.171  40.945  33.774  1.00 22.15
    ATOM   2594 O   PHE A 340  0   -7.069  42.069  33.266  1.00 21.26
20  ATOM   2595 CB  PHE A 340  0   -6.210  39.135  32.397  1.00 22.39
    ATOM   2596 CG  PHE A 340  0   -6.333  37.792  31.736  1.00 20.74
    ATOM   2597 CD1 PHE A 340  0   -6.338  37.710  30.357  1.00 20.97
    ATOM   2598 CD2 PHE A 340  0   -6.448  36.644  32.468  1.00 21.19
    ATOM   2599 CE1 PHE A 340  0   -6.449  36.488  29.721  1.00 21.61
25  ATOM   2600 CE2 PHE A 340  0   -6.585  35.408  31.826  1.00 22.99
    ATOM   2601 CZ  PHE A 340  0   -6.578  35.334  30.444  1.00 19.90
    ATOM   2602 N   THR A 341  0   -7.000  40.736  35.069  1.00 20.76
    ATOM   2603 CA  THR A 341  0   -6.605  41.879  35.889  1.00 21.55
    ATOM   2604 C   THR A 341  0   -5.400  41.509  36.759  1.00 21.00
30  ATOM   2605 O   THR A 341  0   -5.236  40.329  37.089  1.00 20.70
    ATOM   2606 CB  THR A 341  0   -7.757  42.255  36.853  1.00 21.12
    ATOM   2607 OG1 THR A 341  0   -8.014  41.102  37.668  1.00 21.26
    ATOM   2608 CG2 THR A 341  0   -9.050  42.630  36.150  1.00 21.74
    ATOM   2609 N   ILE A 342  0   -4.750  42.529  37.308  1.00 20.28
35  ATOM   2610 CA  ILE A 342  0   -3.739  42.273  38.333  1.00 20.34
    ATOM   2611 C   ILE A 342  0   -4.026  43.212  39.496  1.00 18.92
    ATOM   2612 O   ILE A 342  0   -4.004  44.437  39.327  1.00 16.42
    ATOM   2613 CB  ILE A 342  0   -2.306  42.439  37.820  1.00 21.04
```

```
     ATOM  2614 CG1 ILE A 342  0  -1.337 42.721 38.988 1.00 21.39
     ATOM  2615 CG2 ILE A 342  0  -2.250 43.540 36.800 1.00 24.57
     ATOM  2616 CD1 ILE A 342  0  -0.260 41.661 38.949 1.00 24.53
     ATOM  2617 N   ASN A 343  0  -4.282 42.601 40.650 1.00 17.77
   5 ATOM  2618 CA  ASN A 343  0  -4.702 43.413 41.782 1.00 21.51
     ATOM  2619 C   ASN A 343  0  -5.881 44.287 41.394 1.00 21.43
     ATOM  2620 O   ASN A 343  0  -5.903 45.495 41.598 1.00 20.26
     ATOM  2621 CB  ASN A 343  0  -3.513 44.231 42.356 1.00 22.34
     ATOM  2622 CG  ASN A 343  0  -2.685 43.190 43.073 1.00 25.38
  10 ATOM  2623 OD1 ASN A 343  0  -2.075 42.218 42.598 1.00 26.90
     ATOM  2624 ND2 ASN A 343  0  -2.652 43.238 44.425 1.00 25.34
     ATOM  2625 N   GLY A 344  0  -6.875 43.703 40.730 1.00 23.77
     ATOM  2626 CA  GLY A 344  0  -8.078 44.406 40.324 1.00 25.28
     ATOM  2627 C   GLY A 344  0  -7.954 45.280 39.111 1.00 26.82
  15 ATOM  2628 O   GLY A 344  0  -9.029 45.728 38.672 1.00 29.56
     ATOM  2629 N   THR A 345  0  -6.798 45.561 38.527 1.00 26.28
     ATOM  2630 CA  THR A 345  0  -6.766 46.440 37.366 1.00 25.48
     ATOM  2631 C   THR A 345  0  -6.343 45.703 36.109 1.00 26.49
     ATOM  2632 O   THR A 345  0  -5.385 44.925 36.122 1.00 28.22
  20 ATOM  2633 CB  THR A 345  0  -5.829 47.648 37.589 1.00 26.17
     ATOM  2634 OG1 THR A 345  0  -6.191 48.334 38.788 1.00 25.32
     ATOM  2635 CG2 THR A 345  0  -5.867 48.677 36.462 1.00 24.83
     ATOM  2636 N   ALA A 346  0  -7.017 46.012 35.008 1.00 24.80
     ATOM  2637 CA  ALA A 346  0  -6.768 45.491 33.688 1.00 23.82
  25 ATOM  2638 C   ALA A 346  0  -5.862 46.511 32.997 1.00 23.77
     ATOM  2639 O   ALA A 346  0  -6.098 47.711 33.088 1.00 22.93
     ATOM  2640 CB  ALA A 346  0  -8.031 45.353 32.841 1.00 24.13
     ATOM  2641 N   TYR A 347  0  -4.793 46.023 32.392 1.00 22.69
     ATOM  2642 CA  TYR A 347  0  -3.862 46.949 31.792 1.00 22.75
  30 ATOM  2643 C   TYR A 347  0  -4.483 47.532 30.527 1.00 23.42
     ATOM  2644 O   TYR A 347  0  -4.954 46.753 29.709 1.00 22.19
     ATOM  2645 CB  TYR A 347  0  -2.521 46.274 31.455 1.00 21.25
     ATOM  2646 CG  TYR A 347  0  -1.584 47.221 30.732 1.00 18.93
     ATOM  2647 CD1 TYR A 347  0  -0.819 48.137 31.442 1.00 18.17
  35 ATOM  2648 CD2 TYR A 347  0  -1.473 47.176 29.353 1.00 19.30
     ATOM  2649 CE1 TYR A 347  0   0.034 49.003 30.763 1.00 18.37
     ATOM  2650 CE2 TYR A 347  0  -0.650 48.063 28.664 1.00 18.40
     ATOM  2651 CZ  TYR A 347  0   0.102 48.962 29.394 1.00 18.99
```

```
    ATOM  2652 OH  TYR A 347 0   0.947 49.802 28.706 1.00 19.65
    ATOM  2653 N   GLU A 348 0  -4.378 48.833 30.359 1.00 25.22
    ATOM  2654 CA  GLU A 348 0  -4.769 49.453 29.098 1.00 28.77
    ATOM  2655 C   GLU A 348 0  -3.659 50.470 28.805 1.00 27.38
 5  ATOM  2656 O   GLU A 348 0  -3.297 51.229 29.704 1.00 28.49
    ATOM  2657 CB  GLU A 348 0  -6.114 50.134 29.110 1.00 32.95
    ATOM  2658 CG  GLU A 348 0  -7.391 49.302 29.072 1.00 39.29
    ATOM  2659 CD  GLU A 348 0  -8.562 50.170 29.559 1.00 43.20
    ATOM  2660 OE1 GLU A 348 0  -8.825 51.211 28.900 1.00 45.31
10  ATOM  2661 OE2 GLU A 348 0  -9.175 49.855 30.601 1.00 44.11
    ATOM  2662 N   SER A 349 0  -3.168 50.541 27.621 1.00 25.73
    ATOM  2663 CA  SER A 349 0  -2.080 51.410 27.201 1.00 28.25
    ATOM  2664 C   SER A 349 0  -2.401 52.887 27.194 1.00 28.71
    ATOM  2665 O   SER A 349 0  -3.279 53.399 26.526 1.00 29.13
15  ATOM  2666 CB  SER A 349 0  -1.743 50.818 25.838 1.00 28.54
    ATOM  2667 OG  SER A 349 0  -0.850 51.499 25.026 1.00 33.31
    ATOM  2668 N   PRO A 350 0  -1.623 53.700 27.898 1.00 29.56
    ATOM  2669 CA  PRO A 350 0  -1.770 55.145 27.997 1.00 28.53
    ATOM  2670 C   PRO A 350 0  -1.480 55.825 26.679 1.00 28.01
20  ATOM  2671 O   PRO A 350 0  -0.787 55.217 25.856 1.00 26.93
    ATOM  2672 CB  PRO A 350 0  -0.752 55.632 29.063 1.00 27.91
    ATOM  2673 CG  PRO A 350 0   0.309 54.560 28.863 1.00 28.03
    ATOM  2674 CD  PRO A 350 0  -0.461 53.245 28.688 1.00 28.76
    ATOM  2675 N   SER A 351 0  -1.951 57.066 26.485 1.00 28.89
25  ATOM  2676 CA  SER A 351 0  -1.630 57.718 25.206 1.00 29.67
    ATOM  2677 C   SER A 351 0  -0.213 58.287 25.257 1.00 27.67
    ATOM  2678 O   SER A 351 0   0.320 58.524 24.177 1.00 28.18
    ATOM  2679 CB  SER A 351 0  -2.566 58.860 24.790 1.00 31.71
    ATOM  2680 OG  SER A 351 0  -2.793 59.679 25.938 1.00 34.19
30  ATOM  2681 N   VAL A 352 0   0.316 58.529 26.449 1.00 25.32
    ATOM  2682 CA  VAL A 352 0   1.703 58.997 26.534 1.00 25.27
    ATOM  2683 C   VAL A 352 0   2.503 57.872 27.211 1.00 23.63
    ATOM  2684 O   VAL A 352 0   2.181 57.493 28.323 1.00 23.26
    ATOM  2685 CB  VAL A 352 0   1.934 60.300 27.303 1.00 24.91
35  ATOM  2686 CG1 VAL A 352 0   1.129 61.436 26.658 1.00 24.41
    ATOM  2687 CG2 VAL A 352 0   3.424 60.635 27.281 1.00 23.35
    ATOM  2688 N   PRO A 353 0   3.498 57.375 26.510 1.00 22.39
    ATOM  2689 CA  PRO A 353 0   4.342 56.300 26.983 1.00 21.86
```

```
    ATOM  2690 C   PRO A 353  0   4.978 56.699 28.300 1.00 20.91
    ATOM  2691 O   PRO A 353  0   5.393 57.852 28.483 1.00 21.91
    ATOM  2692 CB  PRO A 353  0   5.417 56.054 25.916 1.00 23.95
    ATOM  2693 CG  PRO A 353  0   5.181 57.123 24.878 1.00 23.79
  5 ATOM  2694 CD  PRO A 353  0   3.882 57.848 25.180 1.00 23.03
    ATOM  2695 N   THR A 354  0   5.043 55.778 29.234 1.00 18.66
    ATOM  2696 CA  THR A 354  0   5.646 56.015 30.530 1.00 18.05
    ATOM  2697 C   THR A 354  0   6.981 56.739 30.478 1.00 18.33
    ATOM  2698 O   THR A 354  0   7.168 57.630 31.319 1.00 19.46
 10 ATOM  2699 CB  THR A 354  0   5.871 54.661 31.242 1.00 17.10
    ATOM  2700 OG1 THR A 354  0   4.903 53.710 30.797 1.00 17.24
    ATOM  2701 CG2 THR A 354  0   5.772 54.852 32.741 1.00 16.43
    ATOM  2702 N   LEU A 355  0   7.940 56.380 29.618 1.00 17.49
    ATOM  2703 CA  LEU A 355  0   9.215 57.076 29.604 1.00 18.84
 15 ATOM  2704 C   LEU A 355  0   9.013 58.579 29.284 1.00 19.80
    ATOM  2705 O   LEU A 355  0   9.722 59.417 29.849 1.00 17.13
    ATOM  2706 CB  LEU A 355  0  10.200 56.498 28.622 1.00 17.89
    ATOM  2707 CG  LEU A 355  0  11.703 56.488 28.819 1.00 18.66
    ATOM  2708 CD1 LEU A 355  0  12.436 56.851 27.547 1.00 18.37
 20 ATOM  2709 CD2 LEU A 355  0  12.199 57.204 30.056 1.00 16.79
    ATOM  2710 N   LEU A 356  0   8.134 58.883 28.328 1.00 20.48
    ATOM  2711 CA  LEU A 356  0   7.812 60.274 27.993 1.00 21.62
    ATOM  2712 C   LEU A 356  0   7.085 60.932 29.163 1.00 21.28
    ATOM  2713 O   LEU A 356  0   7.497 62.042 29.506 1.00 22.01
 25 ATOM  2714 CB  LEU A 356  0   7.028 60.474 26.700 1.00 22.08
    ATOM  2715 CG  LEU A 356  0   6.850 61.939 26.239 1.00 23.98
    ATOM  2716 CD1 LEU A 356  0   8.157 62.709 26.207 1.00 23.11
    ATOM  2717 CD2 LEU A 356  0   6.191 61.985 24.864 1.00 24.74
    ATOM  2718 N   GLN A 357  0   6.219 60.267 29.922 1.00 21.37
 30 ATOM  2719 CA  GLN A 357  0   5.669 60.893 31.120 1.00 21.87
    ATOM  2720 C   GLN A 357  0   6.759 61.254 32.128 1.00 24.12
    ATOM  2721 O   GLN A 357  0   6.674 62.277 32.811 1.00 24.92
    ATOM  2722 CB  GLN A 357  0   4.636 60.015 31.822 1.00 20.63
    ATOM  2723 CG  GLN A 357  0   3.447 59.674 30.906 1.00 19.17
 35 ATOM  2724 CD  GLN A 357  0   2.547 58.643 31.540 1.00 18.85
    ATOM  2725 OE1 GLN A 357  0   2.162 58.748 32.713 1.00 19.06
    ATOM  2726 NE2 GLN A 357  0   2.262 57.600 30.742 1.00 18.49
    ATOM  2727 N   ILE A 358  0   7.735 60.371 32.346 1.00 25.66
```

```
     ATOM  2728 CA  ILE A 358 0    8.822 60.651 33.263 1.00 26.19
     ATOM  2729 C   ILE A 358 0    9.699 61.800 32.762 1.00 27.66
     ATOM  2730 O   ILE A 358 0    9.940 62.725 33.551 1.00 26.65
     ATOM  2731 CB  ILE A 358 0    9.692 59.420 33.578 1.00 24.79
  5  ATOM  2732 CG1 ILE A 358 0    8.807 58.395 34.304 1.00 24.09
     ATOM  2733 CG2 ILE A 358 0   10.865 59.841 34.451 1.00 23.78
     ATOM  2734 CD1 ILE A 358 0    9.251 56.954 34.234 1.00 23.34
     ATOM  2735 N   MET A 359 0   10.054 61.844 31.486 1.00 29.63
     ATOM  2736 CA  MET A 359 0   10.893 62.910 30.965 1.00 33.02
 10  ATOM  2737 C   MET A 359 0   10.174 64.260 31.027 1.00 34.46
     ATOM  2738 O   MET A 359 0   10.801 65.324 31.026 1.00 33.77
     ATOM  2739 CB  MET A 359 0   11.346 62.664 29.537 1.00 35.67
     ATOM  2740 CG  MET A 359 0   12.065 61.403 29.138 1.00 40.75
     ATOM  2741 SD  MET A 359 0   13.764 61.153 29.671 1.00 44.90
 15  ATOM  2742 CE  MET A 359 0   14.594 62.592 29.007 1.00 44.24
     ATOM  2743 N   SER A 360 0    8.835 64.238 31.070 1.00 33.43
     ATOM  2744 CA  SER A 360 0    8.024 65.430 31.088 1.00 32.92
     ATOM  2745 C   SER A 360 0    7.761 65.995 32.474 1.00 33.24
     ATOM  2746 O   SER A 360 0    6.989 66.966 32.556 1.00 34.08
 20  ATOM  2747 CB  SER A 360 0    6.678 65.134 30.393 1.00 31.34
     ATOM  2748 OG  SER A 360 0    6.928 65.109 28.996 1.00 31.06
     ATOM  2749 N   GLY A 361 0    8.288 65.360 33.517 1.00 32.06
     ATOM  2750 CA  GLY A 361 0    8.072 65.868 34.847 1.00 31.80
     ATOM  2751 C   GLY A 361 0    7.487 64.955 35.880 1.00 32.48
 25  ATOM  2752 O   GLY A 361 0    7.420 65.377 37.043 1.00 33.20
     ATOM  2753 N   ALA A 362 0    6.991 63.769 35.535 1.00 33.69
     ATOM  2754 CA  ALA A 362 0    6.406 62.926 36.601 1.00 35.10
     ATOM  2755 C   ALA A 362 0    7.475 62.615 37.650 1.00 34.45
     ATOM  2756 O   ALA A 362 0    8.598 62.306 37.286 1.00 33.60
 30  ATOM  2757 CB  ALA A 362 0    5.789 61.658 36.043 1.00 34.88
     ATOM  2758 N   GLN A 363 0    7.146 62.676 38.920 1.00 36.22
     ATOM  2759 CA  GLN A 363 0    8.083 62.458 40.007 1.00 37.87
     ATOM  2760 C   GLN A 363 0    7.776 61.189 40.787 1.00 37.20
     ATOM  2761 O   GLN A 363 0    8.620 60.777 41.587 1.00 36.79
 35  ATOM  2762 CB  GLN A 363 0    8.012 63.619 41.022 1.00 40.41
     ATOM  2763 CG  GLN A 363 0    8.986 64.740 40.721 1.00 44.07
     ATOM  2764 CD  GLN A 363 0    8.586 66.154 41.092 1.00 45.77
     ATOM  2765 OE1 GLN A 363 0    7.697 66.473 41.901 1.00 46.53
```

```
   ATOM   2766  NE2 GLN A 363  0    9.294  67.089  40.435  1.00 46.12
   ATOM   2767  N   SER A 364  0    6.579  60.632  40.610  1.00 35.74
   ATOM   2768  CA  SER A 364  0    6.249  59.434  41.381  1.00 34.54
   ATOM   2769  C   SER A 364  0    5.225  58.588  40.653  1.00 34.32
 5 ATOM   2770  O   SER A 364  0    4.605  59.037  39.692  1.00 33.71
   ATOM   2771  CB  SER A 364  0    5.774  59.835  42.769  1.00 35.68
   ATOM   2772  OG  SER A 364  0    4.396  60.095  42.928  1.00 35.86
   ATOM   2773  N   ALA A 365  0    5.015  57.372  41.146  1.00 33.95
   ATOM   2774  CA  ALA A 365  0    4.017  56.486  40.564  1.00 34.62
10 ATOM   2775  C   ALA A 365  0    2.637  57.148  40.560  1.00 34.46
   ATOM   2776  O   ALA A 365  0    1.906  56.995  39.582  1.00 34.37
   ATOM   2777  CB  ALA A 365  0    3.963  55.155  41.301  1.00 33.51
   ATOM   2778  N   ASN A 366  0    2.261  57.916  41.571  1.00 34.45
   ATOM   2779  CA  ASN A 366  0    1.003  58.619  41.632  1.00 36.37
15 ATOM   2780  C   ASN A 366  0    0.708  59.524  40.447  1.00 35.60
   ATOM   2781  O   ASN A 366  0   -0.462  59.719  40.131  1.00 36.50
   ATOM   2782  CB  ASN A 366  0    0.904  59.464  42.918  1.00 38.72
   ATOM   2783  CG  ASN A 366  0    0.794  58.558  44.126  1.00 41.08
   ATOM   2784  OD1 ASN A 366  0    0.863  58.966  45.284  1.00 43.39
20 ATOM   2785  ND2 ASN A 366  0    0.646  57.256  43.914  1.00 42.72
   ATOM   2786  N   ASP A 367  0    1.694  60.046  39.752  1.00 34.06
   ATOM   2787  CA  ASP A 367  0    1.571  60.899  38.610  1.00 33.37
   ATOM   2788  C   ASP A 367  0    1.566  60.122  37.293  1.00 32.09
   ATOM   2789  O   ASP A 367  0    1.430  60.762  36.247  1.00 31.74
25 ATOM   2790  CB  ASP A 367  0    2.768  61.841  38.483  1.00 35.96
   ATOM   2791  CG  ASP A 367  0    3.048  62.818  39.602  1.00 37.69
   ATOM   2792  OD1 ASP A 367  0    2.123  63.209  40.336  1.00 37.23
   ATOM   2793  OD2 ASP A 367  0    4.258  63.194  39.705  1.00 39.62
   ATOM   2794  N   LEU A 368  0    1.791  58.814  37.371  1.00 30.39
30 ATOM   2795  CA  LEU A 368  0    1.897  58.055  36.123  1.00 28.74
   ATOM   2796  C   LEU A 368  0    0.586  57.386  35.745  1.00 28.85
   ATOM   2797  O   LEU A 368  0   -0.214  56.947  36.555  1.00 28.17
   ATOM   2798  CB  LEU A 368  0    3.043  57.046  36.194  1.00 26.94
   ATOM   2799  CG  LEU A 368  0    4.436  57.668  36.422  1.00 27.05
35 ATOM   2800  CD1 LEU A 368  0    5.455  56.581  36.765  1.00 25.41
   ATOM   2801  CD2 LEU A 368  0    4.882  58.499  35.236  1.00 24.44
   ATOM   2802  N   LEU A 369  0    0.392  57.332  34.446  1.00 28.81
   ATOM   2803  CA  LEU A 369  0   -0.753  56.671  33.834  1.00 29.65
```

```
   ATOM  2804  C   LEU A 369  0  -0.238  55.398  33.162  1.00  28.29
   ATOM  2805  O   LEU A 369  0   0.875  55.356  32.660  1.00  25.59
   ATOM  2806  CB  LEU A 369  0  -1.333  57.668  32.821  1.00  30.27
   ATOM  2807  CG  LEU A 369  0  -1.800  58.998  33.456  1.00  32.06
 5 ATOM  2808  CD1 LEU A 369  0  -2.220  59.979  32.370  1.00  31.87
   ATOM  2809  CD2 LEU A 369  0  -2.932  58.787  34.455  1.00  30.89
   ATOM  2810  N   PRO A 370  0  -1.054  54.361  33.157  1.00  27.87
   ATOM  2811  CA  PRO A 370  0  -2.396  54.379  33.688  1.00  26.71
   ATOM  2812  C   PRO A 370  0  -2.513  54.112  35.169  1.00  26.73
10 ATOM  2813  O   PRO A 370  0  -1.872  53.184  35.668  1.00  26.55
   ATOM  2814  CB  PRO A 370  0  -3.126  53.222  32.958  1.00  27.28
   ATOM  2815  CG  PRO A 370  0  -2.003  52.317  32.557  1.00  27.38
   ATOM  2816  CD  PRO A 370  0  -0.720  53.102  32.482  1.00  27.24
   ATOM  2817  N   ALA A 371  0  -3.414  54.810  35.870  1.00  26.16
15 ATOM  2818  CA  ALA A 371  0  -3.581  54.556  37.302  1.00  25.73
   ATOM  2819  C   ALA A 371  0  -3.892  53.103  37.616  1.00  24.59
   ATOM  2820  O   ALA A 371  0  -4.758  52.533  36.946  1.00  25.05
   ATOM  2821  CB  ALA A 371  0  -4.718  55.394  37.903  1.00  26.42
   ATOM  2822  N   GLY A 372  0  -3.261  52.524  38.625  1.00  22.47
20 ATOM  2823  CA  GLY A 372  0  -3.519  51.187  39.087  1.00  21.06
   ATOM  2824  C   GLY A 372  0  -2.691  50.096  38.427  1.00  23.01
   ATOM  2825  O   GLY A 372  0  -2.758  48.928  38.831  1.00  23.85
   ATOM  2826  N   SER A 373  0  -1.910  50.428  37.421  1.00  23.30
   ATOM  2827  CA  SER A 373  0  -1.054  49.459  36.736  1.00  24.36
25 ATOM  2828  C   SER A 373  0   0.429  49.746  36.919  1.00  24.76
   ATOM  2829  O   SER A 373  0   1.257  49.103  36.270  1.00  25.75
   ATOM  2830  CB  SER A 373  0  -1.371  49.584  35.233  1.00  23.25
   ATOM  2831  OG  SER A 373  0  -2.638  49.014  34.952  1.00  23.80
   ATOM  2832  N   VAL A 374  0   0.779  50.799  37.657  1.00  23.87
30 ATOM  2833  CA  VAL A 374  0   2.176  51.255  37.706  1.00  22.95
   ATOM  2834  C   VAL A 374  0   2.739  51.109  39.105  1.00  21.72
   ATOM  2835  O   VAL A 374  0   2.093  51.518  40.059  1.00  21.03
   ATOM  2836  CB  VAL A 374  0   2.317  52.687  37.169  1.00  23.05
   ATOM  2837  CG1 VAL A 374  0   3.720  53.273  37.323  1.00  24.13
35 ATOM  2838  CG2 VAL A 374  0   1.945  52.771  35.698  1.00  21.58
   ATOM  2839  N   TYR A 375  0   3.862  50.402  39.246  1.00  20.52
   ATOM  2840  CA  TYR A 375  0   4.445  50.184  40.573  1.00  22.02
   ATOM  2841  C   TYR A 375  0   5.873  50.743  40.549  1.00  22.56
```

```
    ATOM 2842 O   TYR A 375 0   6.665 50.524 39.639 1.00 21.82
    ATOM 2843 CB  TYR A 375 0   4.467 48.729 41.067 1.00 21.98
    ATOM 2844 CG  TYR A 375 0   3.042 48.217 41.226 1.00 24.04
    ATOM 2845 CD1 TYR A 375 0   2.398 48.261 42.445 1.00 23.57
  5 ATOM 2846 CD2 TYR A 375 0   2.339 47.760 40.115 1.00 24.92
    ATOM 2847 CE1 TYR A 375 0   1.100 47.831 42.575 1.00 25.65
    ATOM 2848 CE2 TYR A 375 0   1.034 47.327 40.220 1.00 25.89
    ATOM 2849 CZ  TYR A 375 0   0.429 47.352 41.464 1.00 26.65
    ATOM 2850 OH  TYR A 375 0  -0.869 46.916 41.593 1.00 27.26
 10 ATOM 2851 N   GLU A 376 0   6.130 51.563 41.546 1.00 22.36
    ATOM 2852 CA  GLU A 376 0   7.403 52.214 41.718 1.00 23.62
    ATOM 2853 C   GLU A 376 0   8.411 51.289 42.387 1.00 22.40
    ATOM 2854 O   GLU A 376 0   8.062 50.578 43.324 1.00 21.88
    ATOM 2855 CB  GLU A 376 0   7.211 53.465 42.614 1.00 25.13
 15 ATOM 2856 CG  GLU A 376 0   8.500 54.255 42.720 1.00 27.91
    ATOM 2857 CD  GLU A 376 0   8.376 55.725 43.046 1.00 29.20
    ATOM 2858 OE1 GLU A 376 0   7.247 56.268 43.109 1.00 30.01
    ATOM 2859 OE2 GLU A 376 0   9.458 56.336 43.219 1.00 28.05
    ATOM 2860 N   LEU A 377 0   9.669 51.353 41.954 1.00 21.23
 20 ATOM 2861 CA  LEU A 377 0  10.705 50.535 42.626 1.00 19.95
    ATOM 2862 C   LEU A 377 0  11.838 51.478 42.982 1.00 20.30
    ATOM 2863 O   LEU A 377 0  12.220 52.350 42.197 1.00 20.12
    ATOM 2864 CB  LEU A 377 0  11.129 49.419 41.692 1.00 20.77
    ATOM 2865 CG  LEU A 377 0  10.668 47.964 41.818 1.00 20.49
 25 ATOM 2866 CD1 LEU A 377 0   9.439 47.739 42.629 1.00 17.77
    ATOM 2867 CD2 LEU A 377 0  10.617 47.242 40.483 1.00 19.28
    ATOM 2868 N   PRO A 378 0  12.407 51.334 44.162 1.00 19.69
    ATOM 2869 CA  PRO A 378 0  13.523 52.117 44.631 1.00 19.91
    ATOM 2870 C   PRO A 378 0  14.797 51.650 43.937 1.00 19.81
 30 ATOM 2871 O   PRO A 378 0  14.795 50.645 43.241 1.00 17.74
    ATOM 2872 CB  PRO A 378 0  13.611 51.893 46.157 1.00 20.21
    ATOM 2873 CG  PRO A 378 0  12.957 50.546 46.291 1.00 20.73
    ATOM 2874 CD  PRO A 378 0  12.050 50.292 45.114 1.00 19.74
    ATOM 2875 N   ARG A 379 0  15.877 52.410 44.059 1.00 19.68
 35 ATOM 2876 CA  ARG A 379 0  17.172 52.135 43.449 1.00 18.58
    ATOM 2877 C   ARG A 379 0  18.027 51.129 44.193 1.00 18.68
    ATOM 2878 O   ARG A 379 0  18.151 51.126 45.432 1.00 17.60
    ATOM 2879 CB  ARG A 379 0  17.946 53.487 43.431 1.00 18.33
```

```
   ATOM 2880 CG  ARG A 379 0   19.406 53.348 43.030 1.00 19.33
   ATOM 2881 CD  ARG A 379 0   20.026 54.710 42.729 1.00 19.06
   ATOM 2882 NE  ARG A 379 0   21.413 54.561 42.295 1.00 16.65
   ATOM 2883 CZ  ARG A 379 0   21.794 54.681 41.031 1.00 15.60
 5 ATOM 2884 NH1 ARG A 379 0   20.964 54.904 40.038 1.00 14.29
   ATOM 2885 NH2 ARG A 379 0   23.096 54.505 40.783 1.00 17.29
   ATOM 2886 N   ASN A 380 0   18.701 50.263 43.441 1.00 20.11
   ATOM 2887 CA  ASN A 380 0   19.658 49.328 44.011 1.00 21.97
   ATOM 2888 C   ASN A 380 0   19.129 48.604 45.227 1.00 22.44
10 ATOM 2889 O   ASN A 380 0   19.712 48.630 46.317 1.00 22.53
   ATOM 2890 CB  ASN A 380 0   20.995 50.045 44.345 1.00 23.30
   ATOM 2891 CG  ASN A 380 0   21.860 50.231 43.107 1.00 25.83
   ATOM 2892 OD1 ASN A 380 0   22.636 51.186 42.877 1.00 27.14
   ATOM 2893 ND2 ASN A 380 0   21.767 49.271 42.185 1.00 24.91
15 ATOM 2894 N   GLN A 381 0   17.974 47.936 45.097 1.00 21.39
   ATOM 2895 CA  GLN A 381 0   17.468 47.162 46.220 1.00 20.88
   ATOM 2896 C   GLN A 381 0   17.169 45.760 45.679 1.00 19.96
   ATOM 2897 O   GLN A 381 0   17.000 45.635 44.471 1.00 19.90
   ATOM 2898 CB  GLN A 381 0   16.219 47.722 46.871 1.00 22.84
20 ATOM 2899 CG  GLN A 381 0   16.326 49.172 47.318 1.00 27.28
   ATOM 2900 CD  GLN A 381 0   16.065 49.297 48.792 1.00 30.24
   ATOM 2901 OE1 GLN A 381 0   15.067 49.917 49.171 1.00 34.48
   ATOM 2902 NE2 GLN A 381 0   16.929 48.742 49.611 1.00 30.80
   ATOM 2903 N   VAL A 382 0   17.046 44.825 46.594 1.00 18.67
25 ATOM 2904 CA  VAL A 382 0   16.665 43.472 46.248 1.00 18.98
   ATOM 2905 C   VAL A 382 0   15.139 43.327 46.212 1.00 19.75
   ATOM 2906 O   VAL A 382 0   14.443 43.550 47.225 1.00 18.76
   ATOM 2907 CB  VAL A 382 0   17.252 42.491 47.278 1.00 19.03
   ATOM 2908 CG1 VAL A 382 0   16.811 41.065 46.960 1.00 18.87
30 ATOM 2909 CG2 VAL A 382 0   18.779 42.637 47.344 1.00 17.54
   ATOM 2910 N   VAL A 383 0   14.601 42.954 45.046 1.00 17.58
   ATOM 2911 CA  VAL A 383 0   13.151 42.715 45.037 1.00 17.76
   ATOM 2912 C   VAL A 383 0   12.777 41.254 44.883 1.00 17.50
   ATOM 2913 O   VAL A 383 0   13.348 40.472 44.153 1.00 16.42
35 ATOM 2914 CB  VAL A 383 0   12.306 43.626 44.145 1.00 17.69
   ATOM 2915 CG1 VAL A 383 0   13.111 44.759 43.585 1.00 15.33
   ATOM 2916 CG2 VAL A 383 0   11.400 43.009 43.126 1.00 17.79
   ATOM 2917 N   GLU A 384 0   11.743 40.861 45.638 1.00 18.47
```

```
      ATOM  2918 CA  GLU A 384 0   11.173 39.529 45.542 1.00 18.27
      ATOM  2919 C   GLU A 384 0    9.711 39.683 45.096 1.00 18.94
      ATOM  2920 O   GLU A 384 0    8.956 40.311 45.816 1.00 19.06
      ATOM  2921 CB  GLU A 384 0   11.253 38.764 46.852 1.00 17.12
   5  ATOM  2922 CG  GLU A 384 0   10.717 37.345 46.738 1.00 17.52
      ATOM  2923 CD  GLU A 384 0   10.979 36.551 47.998 1.00 19.10
      ATOM  2924 OE1 GLU A 384 0   12.101 36.050 48.218 1.00 20.69
      ATOM  2925 OE2 GLU A 384 0   10.018 36.405 48.773 1.00 21.22
      ATOM  2926 N   LEU A 385 0    9.326 39.182 43.948 1.00 19.78
  10  ATOM  2927 CA  LEU A 385 0    7.966 39.153 43.463 1.00 21.07
      ATOM  2928 C   LEU A 385 0    7.391 37.738 43.591 1.00 20.91
      ATOM  2929 O   LEU A 385 0    8.043 36.790 43.113 1.00 21.40
      ATOM  2930 CB  LEU A 385 0    7.881 39.466 41.959 1.00 20.92
      ATOM  2931 CG  LEU A 385 0    8.393 40.795 41.457 1.00 23.75
  15  ATOM  2932 CD1 LEU A 385 0    8.118 40.984 39.962 1.00 23.01
      ATOM  2933 CD2 LEU A 385 0    7.827 41.977 42.244 1.00 22.40
      ATOM  2934 N   VAL A 386 0    6.182 37.574 44.099 1.00 20.91
      ATOM  2935 CA  VAL A 386 0    5.510 36.274 44.189 1.00 19.03
      ATOM  2936 C   VAL A 386 0    4.228 36.334 43.356 1.00 21.11
  20  ATOM  2937 O   VAL A 386 0    3.465 37.326 43.516 1.00 20.56
      ATOM  2938 CB  VAL A 386 0    5.159 35.967 45.654 1.00 20.91
      ATOM  2939 CG1 VAL A 386 0    4.518 34.575 45.739 1.00 20.40
      ATOM  2940 CG2 VAL A 386 0    6.321 36.044 46.625 1.00 19.89
      ATOM  2941 N   VAL A 387 0    4.011 35.469 42.358 1.00 20.02
  25  ATOM  2942 CA  VAL A 387 0    2.817 35.515 41.491 1.00 20.83
      ATOM  2943 C   VAL A 387 0    2.119 34.152 41.385 1.00 21.15
      ATOM  2944 O   VAL A 387 0    2.369 33.285 40.528 1.00 19.97
      ATOM  2945 CB  VAL A 387 0    3.163 36.076 40.104 1.00 20.91
      ATOM  2946 CG1 VAL A 387 0    1.917 36.472 39.297 1.00 22.49
  30  ATOM  2947 CG2 VAL A 387 0    3.959 37.393 40.171 1.00 22.24
      ATOM  2948 N   PRO A 388 0    1.262 33.832 42.358 1.00 20.55
      ATOM  2949 CA  PRO A 388 0    0.570 32.548 42.483 1.00 20.93
      ATOM  2950 C   PRO A 388 0   -0.271 32.226 41.264 1.00 20.76
      ATOM  2951 O   PRO A 388 0   -0.928 33.118 40.715 1.00 19.53
  35  ATOM  2952 CB  PRO A 388 0   -0.310 32.559 43.757 1.00 20.54
      ATOM  2953 CG  PRO A 388 0    0.280 33.766 44.482 1.00 21.86
      ATOM  2954 CD  PRO A 388 0    0.841 34.707 43.438 1.00 20.83
      ATOM  2955 N   ALA A 389 0   -0.160 30.986 40.807 1.00 21.68
```

ATOM   2956 CA ALA A 389 0 -0.983 30.617 39.640 1.00 24.20
ATOM   2957 C   ALA A 389 0 -2.394 30.320 40.148 1.00 25.02
ATOM   2958 O   ALA A 389 0 -2.619 30:162 41.350 1.00 24.19
ATOM   2959 CB ALA A 389 0 -0.383 29.403 38.968 1.00 23.67
5 ATOM 2960 N   GLY A 390 0 -3.309 30.143 39.222 1.00 28.43
ATOM   2961 CA GLY A 390 0 -4.713 29.811 39.539 1.00 28.47
ATOM   2962 C   GLY A 390 0 -5.624 30.325 38.431 1.00 28.63
ATOM   2963 O   GLY A 390 0 -6.512 29.630 37.937 1.00 31.26
ATOM   2964 N   VAL A 391 0 -5.402 31.531 37.961 1.00 27.11
10 ATOM 2965 CA VAL A 391 0 -6.234 32.164 36.962 1.00 26.51
ATOM   2966 C   VAL A 391 0 -6.246 31.377 35.666 1.00 29.59
ATOM   2967 O   VAL A 391 0 -5.274 30.775 35.181 1.00 30.61
ATOM   2968 CB VAL A 391 0 -5.835 33.634 36.788 1.00 25.83
ATOM   2969 CG1 VAL A 391 0 -4.584 33.787 35.937 1.00 24.18
15 ATOM 2970 CG2 VAL A 391 0 -7.017 34.419 36.219 1.00 24.11
ATOM   2971 N   LEU A 392 0 -7.439 31.392 35.058 1.00 30.83
ATOM   2972 CA LEU A 392 0 -7.705 30.604 33.867 1.00 30.29
ATOM   2973 C   LEU A 392 0 -6.809 31.004 32.710 1.00 27.38
ATOM   2974 O   LEU A 392 0 -6.316 32.113 32.665 1.00 24.62
20 ATOM 2975 CB LEU A 392 0 -9.173 30.726 33.436 1.00 32.58
ATOM   2976 CG LEU A 392 0 -9.711 32.126 33.189 1.00 33.97
ATOM   2977 CD1 LEU A 392 0 -9.411 32.626 31.786 1.00 34.78
ATOM   2978 CD2 LEU A 392 0 -11.225 32.122 33.463 1.00 36.03
ATOM   2979 N   GLY A 393 0 -6.725 30.074 31.754 1.00 26.24
25 ATOM 2980 CA GLY A 393 0 -5.936 30.302 30.554 1.00 25.54
ATOM   2981 C   GLY A 393 0 -4.458 29.994 30.710 1.00 25.81
ATOM   2982 O   GLY A 393 0 -3.686 30.361 29.820 1.00 26.67
ATOM   2983 N   GLY A 394 0 -4.033 29.379 31.803 1.00 25.84
ATOM   2984 CA GLY A 394 0 -2.615 29.112 32.035 1.00 25.94
30 ATOM 2985 C   GLY A 394 0 -2.140 27.844 31.348 1.00 26.00
ATOM   2986 O   GLY A 394 0 -2.884 27.193 30.625 1.00 25.18
ATOM   2987 N   PRO A 395 0 -0.860 27.527 31.517 1.00 24.26
ATOM   2988 CA PRO A 395 0   0.051 28.258 32.364 1.00 21.79
ATOM   2989 C   PRO A 395 0   0.517 29.518 31.660 1.00 19.29
35 ATOM 2990 O   PRO A 395 0   0.704 29.597 30.445 1.00 17.41
ATOM   2991 CB PRO A 395 0   1.159 27.279 32.794 1.00 22.52
ATOM   2992 CG PRO A 395 0   1.062 26.223 31.758 1.00 24.35
ATOM   2993 CD PRO A 395 0 -0.241 26.312 30.973 1.00 24.87

```
    ATOM  2994 N   HIS A 396 0   0.586 30.591 32.451 1.00 16.97
    ATOM  2995 CA  HIS A 396 0   0.970 31.917 31.980 1.00 15.05
    ATOM  2996 C   HIS A 396 0   2.477 32.137 32.186 1.00 15.41
    ATOM  2997 O   HIS A 396 0   3.039 32.025 33.275 1.00 14.21
  5 ATOM  2998 CB  HIS A 396 0   0.288 32.989 32.842 1.00 15.40
    ATOM  2999 CG  HIS A 396 0  -1.224 32.924 32.737 1.00 18.23
    ATOM  3000 ND1 HIS A 396 0  -1.942 33.504 31.702 1.00 16.23
    ATOM  3001 CD2 HIS A 396 0  -2.109 32.319 33.557 1.00 17.00
    ATOM  3002 CE1 HIS A 396 0  -3.218 33.262 31.906 1.00 18.22
 10 ATOM  3003 NE2 HIS A 396 0  -3.343 32.526 33.014 1.00 19.08
    ATOM  3004 N   PRO A 397 0   3.143 32.403 31.090 1.00 14.69
    ATOM  3005 CA  PRO A 397 0   4.593 32.617 31.080 1.00 16.91
    ATOM  3006 C   PRO A 397 0   4.818 34.129 31.202 1.00 17.59
    ATOM  3007 O   PRO A 397 0   4.524 34.843 30.235 1.00 17.59
 15 ATOM  3008 CB  PRO A 397 0   5.076 32.040 29.757 1.00 16.63
    ATOM  3009 CG  PRO A 397 0   3.785 31.844 28.978 1.00 17.83
    ATOM  3010 CD  PRO A 397 0   2.620 32.464 29.736 1.00 14.36
    ATOM  3011 N   PHE A 398 0   5.242 34.590 32.377 1.00 16.39
    ATOM  3012 CA  PHE A 398 0   5.462 36.019 32.529 1.00 15.95
 20 ATOM  3013 C   PHE A 398 0   6.906 36.365 32.168 1.00 15.74
    ATOM  3014 O   PHE A 398 0   7.846 35.619 32.444 1.00 15.78
    ATOM  3015 CB  PHE A 398 0   5.173 36.455 33.963 1.00 17.20
    ATOM  3016 CG  PHE A 398 0   3.817 37.073 34.169 1.00 19.23
    ATOM  3017 CD1 PHE A 398 0   2.673 36.299 34.005 1.00 19.58
 25 ATOM  3018 CD2 PHE A 398 0   3.688 38.403 34.537 1.00 19.42
    ATOM  3019 CE1 PHE A 398 0   1.409 36.832 34.198 1.00 19.83
    ATOM  3020 CE2 PHE A 398 0   2.405 38.933 34.709 1.00 21.46
    ATOM  3021 CZ  PHE A 398 0   1.260 38.162 34.539 1.00 19.65
    ATOM  3022 N   HIS A 399 0   7.080 37.562 31.640 1.00 14.77
 30 ATOM  3023 CA  HIS A 399 0   8.374 38.089 31.333 1.00 14.75
    ATOM  3024 C   HIS A 399 0   8.580 39.496 31.872 1.00 17.67
    ATOM  3025 O   HIS A 399 0   7.635 40.308 31.925 1.00 18.29
    ATOM  3026 CB  HIS A 399 0   8.582 37.968 29.861 1.00 14.01
    ATOM  3027 CG  HIS A 399 0   8.747 39.105 28.962 1.00 16.26
 35 ATOM  3028 ND1 HIS A 399 0   9.957 39.511 28.446 1.00 15.35
    ATOM  3029 CD2 HIS A 399 0   7.788 39.903 28.386 1.00 17.58
    ATOM  3030 CE1 HIS A 399 0   9.764 40.507 27.593 1.00 15.61
    ATOM  3031 NE2 HIS A 399 0   8.457 40.770 27.548 1.00 17.52
```

```
   ATOM  3032 N   LEU A 400  0   9.837 39.771 32.201 1.00 15.57
   ATOM  3033 CA  LEU A 400  0  10.220 41.061 32.745 1.00 16.93
   ATOM  3034 C   LEU A 400  0  11.207 41.732 31.788 1.00 16.51
   ATOM  3035 O   LEU A 400  0  12.268 41.175 31.510 1.00 15.77
 5 ATOM  3036 CB  LEU A 400  0  10.913 40.825 34.084 1.00 18.17
   ATOM  3037 CG  LEU A 400  0  10.877 41.741 35.288 1.00 21.27
   ATOM  3038 CD1 LEU A 400  0  12.130 41.638 36.151 1.00 19.27
   ATOM  3039 CD2 LEU A 400  0  10.536 43.166 34.926 1.00 19.86
   ATOM  3040 N   HIS A 401  0  10.945 42.916 31.321 1.00 14.34
10 ATOM  3041 CA  HIS A 401  0  11.830 43.707 30.508 1.00 16.06
   ATOM  3042 C   HIS A 401  0  12.924 44.300 31.428 1.00 16.15
   ATOM  3043 O   HIS A 401  0  12.644 44.543 32.600 1.00 13.61
   ATOM  3044 CB  HIS A 401  0  11.105 44.884 29.843 1.00 13.27
   ATOM  3045 CG  HIS A 401  0  10.184 44.441 28.751 1.00 14.50
15 ATOM  3046 ND1 HIS A 401  0  10.201 44.973 27.479 1.00 14.96
   ATOM  3047 CD2 HIS A 401  0   9.202 43.492 28.750 1.00 12.35
   ATOM  3048 CE1 HIS A 401  0   9.263 44.387 26.725 1.00 12.61
   ATOM  3049 NE2 HIS A 401  0   8.677 43.507 27.492 1.00 12.41
   ATOM  3050 N   GLY A 402  0  14.103 44.549 30.855 1.00 15.59
20 ATOM  3051 CA  GLY A 402  0  15.152 45.209 31.598 1.00 15.18
   ATOM  3052 C   GLY A 402  0  16.009 44.351 32.510 1.00 15.96
   ATOM  3053 O   GLY A 402  0  16.927 44.898 33.170 1.00 16.30
   ATOM  3054 N   HIS A 403  0  15.618 43.147 32.893 1.00 12.96
   ATOM  3055 CA  HIS A 403  0  16.282 42.337 33.873 1.00 15.00
25 ATOM  3056 C   HIS A 403  0  16.226 40.839 33.586 1.00 15.22
   ATOM  3057 O   HIS A 403  0  15.253 40.381 32.971 1.00 16.16
   ATOM  3058 CB  HIS A 403  0  15.525 42.478 35.227 1.00 14.13
   ATOM  3059 CG  HIS A 403  0  15.571 43.829 35.827 1.00 16.69
   ATOM  3060 ND1 HIS A 403  0  16.604 44.253 36.649 1.00 16.13
30 ATOM  3061 CD2 HIS A 403  0  14.744 44.911 35.659 1.00 15.50
   ATOM  3062 CE1 HIS A 403  0  16.425 45.520 37.002 1.00 15.02
   ATOM  3063 NE2 HIS A 403  0  15.285 45.905 36.430 1.00 16.15
   ATOM  3064 N   ALA A 404  0  17.138 40.054 34.113 1.00 13.71
   ATOM  3065 CA  ALA A 404  0  17.039 38.607 34.158 1.00 12.60
35 ATOM  3066 C   ALA A 404  0  16.771 38.370 35.649 1.00 12.31
   ATOM  3067 O   ALA A 404  0  17.156 39.291 36.373 1.00 13.94
   ATOM  3068 CB  ALA A 404  0  18.249 37.819 33.721 1.00 13.84
   ATOM  3069 N   PHE A 405  0  16.085 37.356 36.126 1.00 12.21
```

```
    ATOM 3070 CA  PHE A 405 0  15.813 37.235 37.559 1.00 11.64
    ATOM 3071 C   PHE A 405 0  16.177 35.821 38.008 1.00 12.55
    ATOM 3072 O   PHE A 405 0  16.196 34.883 37.201 1.00 12.23
    ATOM 3073 CB  PHE A 405 0  14.325 37.487 37.907 1.00 11.82
 5  ATOM 3074 CG  PHE A 405 0  13.382 36.893 36.879 1.00 11.75
    ATOM 3075 CD1 PHE A 405 0  13.030 35.557 36.933 1.00 10.76
    ATOM 3076 CD2 PHE A 405 0  12.917 37.663 35.824 1.00 11.55
    ATOM 3077 CE1 PHE A 405 0  12.189 35.002 35.978 1.00 11.52
    ATOM 3078 CE2 PHE A 405 0  12.087 37.112 34.862 1.00 13.32
10  ATOM 3079 CZ  PHE A 405 0  11.692 35.767 34.946 1.00 11.45
    ATOM 3080 N   SER A 406 0  16.414 35.625 39.288 1.00 12.86
    ATOM 3081 CA  SER A 406 0  16.660 34.286 39.796 1.00 13.43
    ATOM 3082 C   SER A 406 0  15.276 33.712 40.130 1.00 13.49
    ATOM 3083 O   SER A 406 0  14.518 34.375 40.847 1.00 10.13
15  ATOM 3084 CB  SER A 406 0  17.433 34.290 41.123 1.00 13.78
    ATOM 3085 OG  SER A 406 0  18.708 34.834 40.938 1.00 16.72
    ATOM 3086 N   VAL A 407 0  15.100 32.453 39.741 1.00 14.53
    ATOM 3087 CA  VAL A 407 0  13.853 31.777 40.093 1.00 13.90
    ATOM 3088 C   VAL A 407 0  14.160 30.943 41.325 1.00 14.53
20  ATOM 3089 O   VAL A 407 0  14.513 29.753 41.262 1.00 14.62
    ATOM 3090 CB  VAL A 407 0  13.333 30.903 38.941 1.00 16.43
    ATOM 3091 CG1 VAL A 407 0  11.969 30.317 39.341 1.00 16.69
    ATOM 3092 CG2 VAL A 407 0  13.272 31.682 37.626 1.00 14.90
    ATOM 3093 N   VAL A 408 0  13.971 31.544 42.485 1.00 14.32
25  ATOM 3094 CA  VAL A 408 0  14.173 30.947 43.780 1.00 15.47
    ATOM 3095 C   VAL A 408 0  13.115 29.870 44.049 1.00 16.51
    ATOM 3096 O   VAL A 408 0  13.387 28.927 44.812 1.00 17.39
    ATOM 3097 CB  VAL A 408 0  14.280 31.967 44.932 1.00 15.75
    ATOM 3098 CG1 VAL A 408 0  15.345 33.015 44.600 1.00 14.81
30  ATOM 3099 CG2 VAL A 408 0  12.952 32.693 45.189 1.00 15.99
    ATOM 3100 N   ARG A 409 0  11.972 29.940 43.387 1.00 16.28
    ATOM 3101 CA  ARG A 409 0  10.960 28.900 43.570 1.00 17.67
    ATOM 3102 C   ARG A 409 0  10.217 28.757 42.236 1.00 17.09
    ATOM 3103 O   ARG A 409 0   9.585 29.698 41.763 1.00 15.25
35  ATOM 3104 CB  ARG A 409 0   9.993 29.143 44.718 1.00 17.87
    ATOM 3105 CG  ARG A 409 0   8.796 28.188 44.663 1.00 21.12
    ATOM 3106 CD  ARG A 409 0   8.008 28.181 45.945 1.00 22.10
    ATOM 3107 NE  ARG A 409 0   6.801 27.370 45.955 1.00 24.80
```

ATOM 3108 CZ ARG A 409 0   5.918 27.361 46.961 1.00 25.93
ATOM 3109 NH1 ARG A 409 0   4.859 26.569 46.877 1.00 27.14
ATOM 3110 NH2 ARG A 409 0   6.068 28.117 48.046 1.00 25.44
ATOM 3111 N   SER A 410 0 10.366 27.576 41.668 1.00 16.33
5 ATOM 3112 CA SER A 410 0   9.802 27.245 40.373 1.00 18.33
ATOM 3113 C   SER A 410 0   8.406 26.612 40.492 1.00 18.60
ATOM 3114 O   SER A 410 0   7.941 26.223 41.566 1.00 16.94
ATOM 3115 CB SER A 410 0 10.724 26.199 39.705 1.00 19.51
ATOM 3116 OG SER A 410 0 11.718 26.865 38.933 1.00 20.28
10 ATOM 3117 N   ALA A 411 0   7.754 26.551 39.343 1.00 18.19
ATOM 3118 CA ALA A 411 0   6.458 25.899 39.231 1.00 19.76
ATOM 3119 C   ALA A 411 0   6.667 24.406 39.474 1.00 22.62
ATOM 3120 O   ALA A 411 0   7.636 23.759 39.067 1.00 20.97
ATOM 3121 CB ALA A 411 0   5.873 26.075 37.841 1.00 17.13
15 ATOM 3122 N   GLY A 412 0   5.710 23.856 40.229 1.00 26.30
ATOM 3123 CA GLY A 412 0   5.714 22.442 40.558 1.00 27.05
ATOM 3124 C   GLY A 412 0   6.692 22.150 41.677 1.00 29.22
ATOM 3125 O   GLY A 412 0   6.917 20.959 41.944 1.00 32.10
ATOM 3126 N   SER A 413 0   7.293 23.139 42.322 1.00 28.66
20 ATOM 3127 CA SER A 413 0   8.223 22.871 43.400 1.00 28.58
ATOM 3128 C   SER A 413 0   7.757 23.600 44.642 1.00 29.64
ATOM 3129 O   SER A 413 0   7.279 24.735 44.524 1.00 30.66
ATOM 3130 CB SER A 413 0   9.610 23.407 43.015 1.00 30.12
ATOM 3131 OG SER A 413 0 10.484 23.233 44.127 1.00 31.74
25 ATOM 3132 N   SER A 414 0   7.902 23.031 45.819 1.00 29.19
ATOM 3133 CA SER A 414 0   7.523 23.753 47.033 1.00 30.71
ATOM 3134 C   SER A 414 0   8.762 24.124 47.834 1.00 30.51
ATOM 3135 O   SER A 414 0   8.746 24.453 49.017 1.00 31.90
ATOM 3136 CB SER A 414 0   6.612 22.832 47.853 1.00 31.10
30 ATOM 3137 OG SER A 414 0   7.438 21.764 48.299 1.00 34.24
ATOM 3138 N   THR A·415 0   9.919 24.063 47.194 1.00 30.60
ATOM 3139 CA THR A 415 0 11.194 24.336 47.860 1.00 30.60
ATOM 3140 C   THR A 415 0 11.819 25.614 47.291 1.00 27.71
ATOM 3141 O   THR A 415 0 11.582 25.998 46.137 1.00 27.49
35 ATOM 3142 CB THR A 415 0 12.089 23.095 47.747 1.00 32.16
ATOM 3143 OG1 THR A 415 0 13.411 23.441 47.285 1.00 35.60
ATOM 3144 CG2 THR A 415 0 11.599 22.103 46.710 1.00 34.11
ATOM 3145 N   TYR A 416 0 12.662 26.268 48.053 1.00 24.34

```
   ATOM  3146 CA  TYR A 416 0  13.288 27.513 47.621 1.00 25.69
   ATOM  3147 C   TYR A 416 0  14.782 27.297 47.392 1.00 24.69
   ATOM  3148 O   TYR A 416 0  15.364 26.603 48.211 1.00 25.96
   ATOM  3149 CB  TYR A 416 0  13.129 28.633 48.659 1.00 23.79
 5 ATOM  3150 CG  TYR A 416 0  11.690 29.091 48.794 1.00 24.53
   ATOM  3151 CD1 TYR A 416 0  10.789 28.387 49.596 1.00 24.14
   ATOM  3152 CD2 TYR A 416 0  11.230 30.219 48.131 1.00 23.99
   ATOM  3153 CE1 TYR A 416 0   9.474 28.799 49.713 1.00 23.70
   ATOM  3154 CE2 TYR A 416 0   9.922 30.641 48.248 1.00 23.96
10 ATOM  3155 CZ  TYR A 416 0   9.050 29.929 49.054 1.00 23.73
   ATOM  3156 OH  TYR A 416 0   7.744 30.337 49.152 1.00 23.53
   ATOM  3157 N   ASN A 417 0  15.360 27.867 46.353 1.00 22.34
   ATOM  3158 CA  ASN A 417 0  16.810 27.702 46.223 1.00 20.83
   ATOM  3159 C   ASN A 417 0  17.425 29.089 46.092 1.00 20.43
15 ATOM  3160 O   ASN A 417 0  17.247 29.761 45.082 1.00 20.00
   ATOM  3161 CB  ASN A 417 0  17.179 26.763 45.086 1.00 19.72
   ATOM  3162 CG  ASN A 417 0  18.660 26.716 44.758 1.00 19.50
   ATOM  3163 OD1 ASN A 417 0  19.485 27.313 45.465 1.00 20.18
   ATOM  3164 ND2 ASN A 417 0  18.981 26.043 43.660 1.00 17.21
20 ATOM  3165 N   PHE A 418 0  18.153 29.508 47.119 1.00 20.79
   ATOM  3166 CA  PHE A 418 0  18.831 30.797 47.049 1.00 20.77
   ATOM  3167 C   PHE A 418 0  20.314 30.613 46.725 1.00 20.47
   ATOM  3168 O   PHE A 418 0  20.973 31.618 46.517 1.00 19.47
   ATOM  3169 CB  PHE A 418 0  18.764 31.542 48.384 1.00 20.52
25 ATOM  3170 CG  PHE A 418 0  17.332 31.821 48.753 1.00 22.19
   ATOM  3171 CD1 PHE A 418 0  16.644 30.947 49.578 1.00 21.36
   ATOM  3172 CD2 PHE A 418 0  16.697 32.951 48.244 1.00 21.95
   ATOM  3173 CE1 PHE A 418 0  15.320 31.208 49.919 1.00 21.64
   ATOM  3174 CE2 PHE A 418 0  15.386 33.198 48.599 1.00 22.81
30 ATOM  3175 CZ  PHE A 418 0  14.694 32.325 49.419 1.00 22.57
   ATOM  3176 N   VAL A 419 0  20.816 29.380 46.732 1.00 19.72
   ATOM  3177 CA  VAL A 419 0  22.272 29.235 46.564 1.00 19.96
   ATOM  3178 C   VAL A 419 0  22.682 29.261 45.114 1.00 20.65
   ATOM  3179 O   VAL A 419 0  23.634 29.875 44.671 1.00 21.02
35 ATOM  3180 CB  VAL A 419 0  22.708 27.888 47.200 1.00 21.81
   ATOM  3181 CG1 VAL A 419 0  23.954 27.291 46.588 1.00 21.97
   ATOM  3182 CG2 VAL A 419 0  22.885 28.098 48.713 1.00 21.55
   ATOM  3183 N   ASN A 420 0  21.867 28.585 44.327 1.00 19.77
```

```
   ATOM 3184 CA  ASN A 420 0   22.076 28.232 42.967 1.00 21.81
   ATOM 3185 C   ASN A 420 0   21.028 28.263 41.891 1.00 20.21
   ATOM 3186 O   ASN A 420 0   21.046 27.407 41.004 1.00 20.13
   ATOM 3187 CB  ASN A 420 0   22.166 26.587 43.207 1.00 21.91
5  ATOM 3188 CG  ASN A 420 0   23.441 26.231 42.529 1.00 24.12
   ATOM 3189 OD1 ASN A 420 0   23.933 25.113 42.403 1.00 26.75
   ATOM 3190 ND2 ASN A 420 0   24.051 27.318 42.027 1.00 25.42
   ATOM 3191 N   PRO A 421 0   19.987 29.034 42.038 1.00 20.27
   ATOM 3192 CA  PRO A 421 0   18.808 28.951 41.183 1.00 17.57
10 ATOM 3193 C   PRO A 421 0   19.100 29.369 39.778 1.00 15.76
   ATOM 3194 O   PRO A 421 0   19.907 30.281 39.586 1.00 15.13
   ATOM 3195 CB  PRO A 421 0   17.769 29.850 41.894 1.00 19.52
   ATOM 3196 CG  PRO A 421 0   18.674 30.863 42.589 1.00 19.88
   ATOM 3197 CD  PRO A 421 0   19.847 30.057 43.095 1.00 20.45
15 ATOM 3198 N   VAL A 422 0   18.385 28.803 38.820 1.00 15.28
   ATOM 3199 CA  VAL A 422 0   18.502 29.239 37.420 1.00 13.48
   ATOM 3200 C   VAL A 422 0   18.157 30.721 37.397 1.00 14.53
   ATOM 3201 O   VAL A 422 0   17.340 31.208 38.183 1.00 14.44
   ATOM 3202 CB  VAL A 422 0   17.498 28.435 36.585 1.00 15.23
20 ATOM 3203 CG1 VAL A 422 0   16.032 28.747 36.937 1.00 13.85
   ATOM 3204 CG2 VAL A 422 0   17.681 28.514 35.089 1.00 13.26
   ATOM 3205 N   LYS A 423 0   18.691 31.447 36.451 1.00 15.35
   ATOM 3206 CA  LYS A 423 0   18.366 32.831 36.189 1.00 17.23
   ATOM 3207 C   LYS A 423 0   17.759 32.891 34.784 1.00 16.55
25 ATOM 3208 O   LYS A 423 0   18.284 32.189 33.909 1.00 16.92
   ATOM 3209 CB  LYS A 423 0   19.627 33.681 36.174 1.00 19.33
   ATOM 3210 CG  LYS A 423 0   20.118 33.985 37.565 1.00 24.09
   ATOM 3211 CD  LYS A 423 0   21.065 35.206 37.466 1.00 27.32
   ATOM 3212 CE  LYS A 423 0   22.470 34.596 37.263 1.00 28.78
30 ATOM 3213 NZ  LYS A 423 0   23.128 34.482 38.595 1.00 29.50
   ATOM 3214 N   ARG A 424 0   16.630 33.570 34.617 1.00 15.85
   ATOM 3215 CA  ARG A 424 0   16.016 33.592 33.294 1.00 16.20
   ATOM 3216 C   ARG A 424 0   15.235 34.890 33.105 1.00 14.86
   ATOM 3217 O   ARG A 424 0   15.354 35.771 33.959 1.00 14.64
35 ATOM 3218 CB  ARG A 424 0   15.158 32.367 32.994 1.00 16.11
   ATOM 3219 CG  ARG A 424 0   14.036 31.864 33.849 1.00 14.06
   ATOM 3220 CD  ARG A 424 0   13.447 30.506 33.427 1.00 11.65
   ATOM 3221 NE  ARG A 424 0   13.422 30.395 31.961 1.00  9.03
```

```
   ATOM   3222 CZ   ARG A 424  0   13.312 29.234 31.319 1.00 10.63
   ATOM   3223 NH1  ARG A 424  0   13.185 28.133 32.082 1.00 11.02
   ATOM   3224 NH2  ARG A 424  0   13.403 29.213 29.988 1.00  8.52
   ATOM   3225 N    ASP A 425  0   14.519 34.975 31.995 1.00 13.83
 5 ATOM   3226 CA   ASP A 425  0   13.751 36.209 31.752 1.00 15.00
   ATOM   3227 C    ASP A 425  0   12.298 35.929 31.359 1.00 15.65
   ATOM   3228 O    ASP A 425  0   11.474 36.850 31.271 1.00 15.11
   ATOM   3229 CB   ASP A 425  0   14.499 37.130 30.797 1.00 12.96
   ATOM   3230 CG   ASP A 425  0   14.609 36.652 29.371 1.00 14.32
10 ATOM   3231 OD1  ASP A 425  0   13.697 35.957 28.818 1.00 13.30
   ATOM   3232 OD2  ASP A 425  0   15.632 37.003 28.729 1.00 13.76
   ATOM   3233 N    VAL A 426  0   11.883 34.675 31.206 1.00 15.21
   ATOM   3234 CA   VAL A 426  0   10.530 34.229 30.984 1.00 13.92
   ATOM   3235 C    VAL A 426  0   10.247 33.000 31.865 1.00 13.98
15 ATOM   3236 O    VAL A 426  0   10.891 31.965 31.696 1.00 15.56
   ATOM   3237 CB   VAL A 426  0   10.128 33.807 29.567 1.00 12.49
   ATOM   3238 CG1  VAL A 426  0    8.629 33.473 29.531 1.00 13.99
   ATOM   3239 CG2  VAL A 426  0   10.390 34.874 28.536 1.00 12.37
   ATOM   3240 N    VAL A 427  0    9.274 33.090 32.766 1.00 12.82
20 ATOM   3241 CA   VAL A 427  0    8.979 31.969 33.639 1.00 12.27
   ATOM   3242 C    VAL A 427  0    7.495 31.589 33.651 1.00 14.14
   ATOM   3243 O    VAL A 427  0    6.594 32.426 33.682 1.00 14.10
   ATOM   3244 CB   VAL A 427  0    9.458 32.315 35.056 1.00 11.46
   ATOM   3245 CG1  VAL A 427  0    8.732 33.549 35.594 1.00  9.39
25 ATOM   3246 CG2  VAL A 427  0    9.353 31.116 35.982 1.00 10.53
   ATOM   3247 N    SER A 428  0    7.229 30.282 33.622 1.00 13.74
   ATOM   3248 CA   SER A 428  0    5.889 29.766 33.721 1.00 15.16
   ATOM   3249 C    SER A 428  0    5.445 29.878 35.171 1.00 15.48
   ATOM   3250 O    SER A 428  0    6.186 29.505 36.087 1.00 15.38
30 ATOM   3251 CB   SER A 428  0    5.776 28.323 33.206 1.00 16.37
   ATOM   3252 OG   SER A 428  0    4.464 27.821 33.484 1.00 17.00
   ATOM   3253 N    LEU A 429  0    4.246 30.376 35.399 1.00 15.74
   ATOM   3254 CA   LEU A 429  0    3.686 30.489 36.744 1.00 15.73
   ATOM   3255 C    LEU A 429  0    3.035 29.184 37.198 1.00 16.41
35 ATOM   3256 O    LEU A 429  0    2.741 29.041 38.390 1.00 15.74
   ATOM   3257 CB   LEU A 429  0    2.669 31.627 36.886 1.00 14.99
   ATOM   3258 CG   LEU A 429  0    3.155 33.027 36.540 1.00 16.60
   ATOM   3259 CD1  LEU A 429  0    2.043 34.042 36.862 1.00 17.78
```

```
   ATOM  3260 CD2 LEU A 429 0   4.438 33.386 37.281 1.00 16.26
   ATOM  3261 N   GLY A 430 0   2.913 28.218 36.295 1.00 17.70
   ATOM  3262 CA  GLY A 430 0   2.419 26.904 36.701 1.00 19.84
   ATOM  3263 C   GLY A 430 0   0.894 26.836 36.778 1.00 20.72
 5 ATOM  3264 O   GLY A 430 0   0.178 27.498 36.029 1.00 20.89
   ATOM  3265 N   VAL A 431 0   0.428 26.056 37.729 1.00 22.04
   ATOM  3266 CA  VAL A 431 0  -0.956 25.713 37.966 1.00 22.61
   ATOM  3267 C   VAL A 431 0  -1.337 26.028 39.409 1.00 23.06
   ATOM  3268 O   VAL A 431 0  -0.476 26.392 40.218 1.00 22.42
10 ATOM  3269 CB  VAL A 431 0  -1.245 24.193 37.768 1.00 23.03
   ATOM  3270 CG1 VAL A 431 0  -0.795 23.672 36.416 1.00 22.74
   ATOM  3271 CG2 VAL A 431 0  -0.574 23.315 38.820 1.00 22.77
   ATOM  3272 N   THR A 432 0  -2.615 25.835 39.704 1.00 23.88
   ATOM  3273 CA  THR A 432 0  -3.168 26.067 41.041 1.00 24.18
15 ATOM  3274 C   THR A 432 0  -2.324 25.401 42.092 1.00 23.94
   ATOM  3275 O   THR A 432 0  -1.915 24.249 41.909 1.00 24.69
   ATOM  3276 CB  THR A 432 0  -4.625 25.565 41.069 1.00 25.75
   ATOM  3277 OG1 THR A 432 0  -5.336 26.344 40.087 1.00 25.87
   ATOM  3278 CG2 THR A 432 0  -5.319 25.800 42.398 1.00 26.65
20 ATOM  3279 N   GLY A 433 0  -1.924 26.136 43.124 1.00 24.45
   ATOM  3280 CA  GLY A 433 0  -1.035 25.589 44.159 1.00 22.27
   ATOM  3281 C   GLY A 433 0   0.394 26.120 43.983 1.00 23.26
   ATOM  3282 O   GLY A 433 0   1.103 26.212 45.000 1.00 23.30
   ATOM  3283 N   ASP A 434 0   0.833 26.481 42.776 1.00 21.12
25 ATOM  3284 CA  ASP A 434 0   2.192 26.986 42.586 1.00 20.62
   ATOM  3285 C   ASP A 434 0   2.360 28.408 43.126 1.00 22.36
   ATOM  3286 O   ASP A 434 0   1.425 29.225 43.076 1.00 21.24
   ATOM  3287 CB  ASP A 434 0   2.548 27.024 41.087 1.00 18.78
   ATOM  3288 CG  ASP A 434 0   2.827 25.616 40.597 1.00 19.71
30 ATOM  3289 OD1 ASP A 434 0   3.304 24.828 41.409 1.00 20.43
   ATOM  3290 OD2 ASP A 434 0   2.596 25.242 39.432 1.00 21.58
   ATOM  3291 N   GLU A 435 0   3.585 28.721 43.562 1.00 22.08
   ATOM  3292 CA  GLU A 435 0   3.853 30.077 44.068 1.00 23.24
   ATOM  3293 C   GLU A 435 0   5.244 30.512 43.612 1.00 20.24
35 ATOM  3294 O   GLU A 435 0   6.201 30.611 44.372 1.00 19.50
   ATOM  3295 CB  GLU A 435 0   3.659 30.068 45.572 1.00 25.56
   ATOM  3296 CG  GLU A 435 0   3.739 31.409 46.258 1.00 30.52
   ATOM  3297 CD  GLU A 435 0   3.107 31.350 47.657 1.00 35.00
```

```
    ATOM   3298 OE1 GLU A 435 0    2.093 30.603 47.760 1.00 35.71
    ATOM   3299 OE2 GLU A 435 0    3.658 32.020 48.579 1.00 35.91
    ATOM   3300 N   VAL A 436 0    5.344 30.690 42.297 1.00 17.80
    ATOM   3301 CA  VAL A 436 0    6.564 31.083 41.640 1.00 15.30
  5 ATOM   3302 C   VAL A 436 0    7.049 32.416 42.221 1.00 17.15
    ATOM   3303 O   VAL A 436 0    6.326 33.402 42.275 1.00 17.48
    ATOM   3304 CB  VAL A 436 0    6.360 31.219 40.129 1.00 14.63
    ATOM   3305 CG1 VAL A 436 0    7.463 32.009 39.454 1.00 10.79
    ATOM   3306 CG2 VAL A 436 0    6.238 29.806 39.536 1.00 14.13
 10 ATOM   3307 N   THR A 437 0    8.290 32.391 42.691 1.00 16.51
    ATOM   3308 CA  THR A 437 0    8.940 33.505 43.364 1.00 16.19
    ATOM   3309 C   THR A 437 0   10.254 33.817 42.668 1.00 15.24
    ATOM   3310 O   THR A 437 0   11.100 32.940 42.419 1.00 15.47
    ATOM   3311 CB  THR A 437 0    9.190 33.067 44.827 1.00 14.95
 15 ATOM   3312 OG1 THR A 437 0    7.969 32.499 45.308 1.00 13.50
    ATOM   3313 CG2 THR A 437 0    9.599 34.232 45.697 1.00 13.41
    ATOM   3314 N   ILE A 438 0   10.413 35.059 42.251 1.00 13.38
    ATOM   3315 CA  ILE A 438 0   11.597 35.471 41.510 1.00 15.78
    ATOM   3316 C   ILE A 438 0   12.292 36.590 42.264 1.00 15.86
 20 ATOM   3317 O   ILE A 438 0   11.617 37.270 43.048 1.00 17.32
    ATOM   3318 CB  ILE A 438 0   11.249 35.848 40.053 1.00 15.40
    ATOM   3319 CG1 ILE A 438 0   10.340 37.055 39.985 1.00 15.85
    ATOM   3320 CG2 ILE A 438 0   10.602 34.653 39.346 1.00 17.11
    ATOM   3321 CD1 ILE A 438 0    9.971 37.607 38.632 1.00 17.49
 25 ATOM   3322 N   ARG A 439 0   13.599 36.789 42.055 1.00 16.02
    ATOM   3323 CA  ARG A 439 0   14.315 37.896 42.671 1.00 13.90
    ATOM   3324 C   ARG A 439 0   15.181 38.645 41.676 1.00 13.52
    ATOM   3325 O   ARG A 439 0   15.748 38.056 40.762 1.00 14.74
    ATOM   3326 CB  ARG A 439 0   15.193 37.501 43.850 1.00 15.15
 30 ATOM   3327 CG  ARG A 439 0   14.457 37.235 45.147 1.00 14.83
    ATOM   3328 CD  ARG A 439 0   15.367 37.337 46.355 1.00 14.08
    ATOM   3329 NE  ARG A 439 0   14.613 37.000 47.566 1.00 17.06
    ATOM   3330 CZ  ARG A 439 0   15.192 36.922 48.767 1.00 18.01
    ATOM   3331 NH1 ARG A 439 0   16.487 37.176 48.908 1.00 17.76
 35 ATOM   3332 NH2 ARG A 439 0   14.459 36.604 49.818 1.00 18.55
    ATOM   3333 N   PHE A 440 0   15.314 39.957 41.853 1.00 14.44
    ATOM   3334 CA  PHE A 440 0   16.204 40.737 40.993 1.00 15.97
    ATOM   3335 C   PHE A 440 0   16.645 41.986 41.761 1.00 15.86
```

ATOM 3336 O   PHE A 440 0   16.113 42.313 42.801 1.00 15.79
ATOM 3337 CB PHE A 440 0   15.638 41.081 39.620 1.00 15.17
ATOM 3338 CG PHE A 440 0   14.416 41.948 39.647 1.00 16.95
ATOM 3339 CD1 PHE A 440 0   14.525 43.333 39.528 1.00 17.23
5 ATOM 3340 CD2 PHE A 440 0   13.158 41.377 39.798 1.00 16.35
ATOM 3341 CE1 PHE A 440 0   13.397 44.152 39.566 1.00 17.07
ATOM 3342 CE2 PHE A 440 0   12.026 42.180 39.841 1.00 17.12
ATOM 3343 CZ PHE A 440 0   12.144 43.575 39.719 1.00 18.30
ATOM 3344 N   VAL A 441 0   17.676 42.648 41.268 1.00 16.10
10 ATOM 3345 CA VAL A 441 0   18.172 43.874 41.879 1.00 16.29
ATOM 3346 C   VAL A 441 0   17.776 45.035 40.972 1.00 14.00
ATOM 3347 O   VAL A 441 0   17.866 44.924 39.736 1.00 12.72
ATOM 3348 CB VAL A 441 0   19.675 43.769 42.144 1.00 18.13
ATOM 3349 CG1 VAL A 441 0   20.195 45.040 42.794 1.00 18.53
15 ATOM 3350 CG2 VAL A 441 0   19.969 42.583 43.065 1.00 18.55
ATOM 3351 N   THR A 442 0   17.328 46.125 41.579 1.00 11.73
ATOM 3352 CA THR A 442 0   16.905 47.291 40.800 1.00 13.02
ATOM 3353 C   THR A 442 0   18.055 48.208 40.432 1.00 14.83
ATOM 3354 O   THR A 442 0   18.218 49.323 40.947 1.00 15.17
20 ATOM 3355 CB THR A 442 0   15.840 48.127 41.558 1.00 14.62
ATOM 3356 OG1 THR A 442 0   16.314 48.463 42.864 1.00 14.34
ATOM 3357 CG2 THR A 442 0   14.552 47.299 41.727 1.00 13.82
ATOM 3358 N   ASP A 443 0   18.818 47.764 39.437 1.00 15.48
ATOM 3359 CA ASP A 443 0   20.004 48.449 38.964 1.00 16.57
25 ATOM 3360 C   ASP A 443 0   19.807 49.010 37.569 1.00 15.38
ATOM 3361 O   ASP A 443 0   20.788 49.208 36.858 1.00 15.57
ATOM 3362 CB ASP A 443 0   21.133 47.391 38.962 1.00 19.75
ATOM 3363 CG ASP A 443 0   20.877 46.264 37.990 1.00 22.78
ATOM 3364 OD1 ASP A 443 0   21.711 45.353 37.789 1.00 25.70
30 ATOM 3365 OD2 ASP A 443 0   19.836 46.161 37.313 1.00 23.88
ATOM 3366 N   ASN A 444 0   18.593 49.278 37.144 1.00 13.71
ATOM 3367 CA ASN A 444 0   18.388 49.721 35.752 1.00 15.87
ATOM 3368 C   ASN A 444 0   17.245 50.728 35.702 1.00 17.00
ATOM 3369 O   ASN A 444 0   16.052 50.419 35.614 1.00 16.83
35 ATOM 3370 CB ASN A 444 0   18.198 48.453 34.930 1.00 15.78
ATOM 3371 CG ASN A 444 0   18.225 48.675 33.442 1.00 18.49
ATOM 3372 OD1 ASN A 444 0   18.505 49.809 33.047 1.00 19.42
ATOM 3373 ND2 ASN A 444 0   17.925 47.689 32.588 1.00 15.91

```
   ATOM  3374  N   PRO A 445  0   17.598 52.003 35.890 1.00 17.59
   ATOM  3375  CA  PRO A 445  0   16.683 53.137 35.938 1.00 16.56
   ATOM  3376  C   PRO A 445  0   15.788 53.217 34.721 1.00 16.99
   ATOM  3377  O   PRO A 445  0   16.293 53.246 33.594 1.00 17.02
 5 ATOM  3378  CB  PRO A 445  0   17.552 54.418 35.951 1.00 18.28
   ATOM  3379  CG  PRO A 445  0   18.870 53.871 36.474 1.00 18.09
   ATOM  3380  CD  PRO A 445  0   19.002 52.409 36.084 1.00 16.05
   ATOM  3381  N   GLY A 446  0   14.462 53.194 34.918 1.00 17.16
   ATOM  3382  CA  GLY A 446  0   13.560 53.281 33.743 1.00 15.84
10 ATOM  3383  C   GLY A 446  0   12.297 52.453 33.984 1.00 14.24
   ATOM  3384  O   GLY A 446  0   12.192 51.797 35.005 1.00 12.22
   ATOM  3385  N   PRO A 447  0   11.285 52.697 33.181 1.00 15.53
   ATOM  3386  CA  PRO A 447  0    9.999 52.048 33.195 1.00 15.24
   ATOM  3387  C   PRO A 447  0   10.101 50.737 32.401 1.00 13.82
15 ATOM  3388  O   PRO A 447  0   10.514 50.733 31.240 1.00 13.85
   ATOM  3389  CB  PRO A 447  0    9.013 52.976 32.473 1.00 16.21
   ATOM  3390  CG  PRO A 447  0    9.933 53.729 31.554 1.00 16.19
   ATOM  3391  CD  PRO A 447  0   11.347 53.707 32.096 1.00 17.15
   ATOM  3392  N   TRP A 448  0    9.787 49.623 33.021 1.00 11.83
20 ATOM  3393  CA  TRP A 448  0    9.898 48.317 32.371 1.00 14.30
   ATOM  3394  C   TRP A 448  0    8.610 47.493 32.427 1.00 13.12
   ATOM  3395  O   TRP A 448  0    8.013 47.355 33.502 1.00 11.63
   ATOM  3396  CB  TRP A 448  0   10.985 47.483 33.095 1.00 13.17
   ATOM  3397  CG  TRP A 448  0   12.321 48.160 33.124 1.00 14.54
25 ATOM  3398  CD1 TRP A 448  0   12.897 48.728 34.239 1.00 14.19
   ATOM  3399  CD2 TRP A 448  0   13.211 48.382 32.029 1.00 14.38
   ATOM  3400  NE1 TRP A 448  0   14.083 49.290 33.873 1.00 15.02
   ATOM  3401  CE2 TRP A 448  0   14.308 49.095 32.527 1.00 14.41
   ATOM  3402  CE3 TRP A 448  0   13.193 48.053 30.672 1.00 15.39
30 ATOM  3403  CZ2 TRP A 448  0   15.388 49.467 31.729 1.00 14.57
   ATOM  3404  CZ3 TRP A 448  0   14.250 48.446 29.867 1.00 14.92
   ATOM  3405  CH2 TRP A 448  0   15.355 49.135 30.399 1.00 14.93
   ATOM  3406  N   PHE A 449  0    8.231 46.884 31.315 1.00 14.03
   ATOM  3407  CA  PHE A 449  0    7.023 46.039 31.297 1.00 13.60
35 ATOM  3408  C   PHE A 449  0    7.231 44.712 32.016 1.00 15.32
   ATOM  3409  O   PHE A 449  0    8.312 44.093 31.993 1.00 13.66
   ATOM  3410  CB  PHE A 449  0    6.627 45.773 29.845 1.00 16.19
   ATOM  3411  CG  PHE A 449  0    5.221 46.033 29.380 1.00 18.26
```

```
   ATOM  3412 CD1 PHE A 449 0    4.165 46.288 30.226 1.00 17.95
   ATOM  3413 CD2 PHE A 449 0    4.962 46.027 28.011 1.00 20.73
   ATOM  3414 CE1 PHE A 449 0    2.899 46.565 29.745 1.00 18.55
   ATOM  3415 CE2 PHE A 449 0    3.701 46.293 27.503 1.00 20.13
 5 ATOM  3416 CZ  PHE A 449 0    2.664 46.543 28.387 1.00 18.59
   ATOM  3417 N   PHE A 450 0    6.195 44.245 32.715 1.00 12.79
   ATOM  3418 CA  PHE A 450 0    6.119 42.963 33.359 1.00 14.38
   ATOM  3419 C   PHE A 450 0    4.775 42.323 32.952 1.00 15.45
   ATOM  3420 O   PHE A 450 0    3.743 42.812 33.423 1.00 15.30
10 ATOM  3421 CB  PHE A 450 0    6.186 43.041 34.879 1.00 15.06
   ATOM  3422 CG  PHE A 450 0    6.210 41.693 35.555 1.00 15.95
   ATOM  3423 CD1 PHE A 450 0    7.157 40.734 35.204 1.00 16.36
   ATOM  3424 CD2 PHE A 450 0    5.325 41.398 36.570 1.00 15.45
   ATOM  3425 CE1 PHE A 450 0    7.222 39.518 35.855 1.00 13.87
15 ATOM  3426 CE2 PHE A 450 0    5.386 40.187 37.224 1.00 16.10
   ATOM  3427 CZ  PHE A 450 0    6.317 39.236 36.854 1.00 15.90
   ATOM  3428 N   HIS A 451 0    4.737 41.301 32.122 1.00 15.54
   ATOM  3429 CA  HIS A 451 0    3.443 40.841 31.610 1.00 16.24
   ATOM  3430 C   HIS A 451 0    3.461 39.426 31.073 1.00 16.95
20 ATOM  3431 O   HIS A 451 0    4.526 38.860 30.812 1.00 17.42
   ATOM  3432 CB  HIS A 451 0    2.996 41.743 30.435 1.00 14.01
   ATOM  3433 CG  HIS A 451 0    3.921 41.696 29.281 1.00 16.98
   ATOM  3434 ND1 HIS A 451 0    3.791 40.844 28.201 1.00 18.14
   ATOM  3435 CD2 HIS A 451 0    5.058 42.435 29.046 1.00 17.88
25 ATOM  3436 CE1 HIS A 451 0    4.759 41.060 27.337 1.00 17.83
   ATOM  3437 NE2 HIS A 451 0    5.554 42.011 27.842 1.00 18.98
   ATOM  3438 N   CYS A 452 0    2.261 38.863 30.951 1.00 16.78
   ATOM  3439 CA  CYS A 452 0    2.167 37.537 30.388 1.00 16.34
   ATOM  3440 C   CYS A 452 0    2.604 37.623 28.924 1.00 14.77
30 ATOM  3441 O   CYS A 452 0    2.167 38.514 28.188 1.00 13.61
   ATOM  3442 CB  CYS A 452 0    0.727 36.983 30.451 1.00 18.22
   ATOM  3443 SG  CYS A 452 0    0.701 35.325 29.692 1.00 19.80
   ATOM  3444 N   HIS A 453 0    3.388 36.640 28.474 1.00 13.29
   ATOM  3445 CA  HIS A 453 0    3.867 36.716 27.100 1.00 13.19
35 ATOM  3446 C   HIS A 453 0    2.983 35.987 26.099 1.00 13.47
   ATOM  3447 O   HIS A 453 0    3.296 35.974 24.906 1.00 11.93
   ATOM  3448 CB  HIS A 453 0    5.314 36.251 27.033 1.00 13.98
   ATOM  3449 CG  HIS A 453 0    6.124 36.860 25.945 1.00 11.89
```

```
     ATOM  3450  ND1 HIS A 453  0    5.835  36.763  24.612  1.00  10.68
     ATOM  3451  CD2 HIS A 453  0    7.270  37.594  26.072  1.00  12.71
     ATOM  3452  CE1 HIS A 453  0    6.776  37.418  23.923  1.00  12.37
     ATOM  3453  NE2 HIS A 453  0    7.663  37.930  24.793  1.00  13.20
 5   ATOM  3454  N   ILE A 454  0    1.860  35.429  26.549  1.00  15.35
     ATOM  3455  CA  ILE A 454  0    0.849  34.937  25.600  1.00  15.85
     ATOM  3456  C   ILE A 454  0    0.214  36.238  25.089  1.00  18.65
     ATOM  3457  O   ILE A 454  0   -0.452  36.997  25.824  1.00  17.92
     ATOM  3458  CB  ILE A 454  0   -0.156  34.001  26.280  1.00  16.46
10   ATOM  3459  CG1 ILE A 454  0    0.456  32.598  26.512  1.00  15.26
     ATOM  3460  CG2 ILE A 454  0   -1.402  33.898  25.419  1.00  14.21
     ATOM  3461  CD1 ILE A 454  0   -0.249  31.804  27.592  1.00  16.26
     ATOM  3462  N   GLU A 455  0    0.448  36.607  23.832  1.00  21.02
     ATOM  3463  CA  GLU A 455  0   -0.024  37.856  23.289  1.00  23.78
15   ATOM  3464  C   GLU A 455  0   -1.526  38.042  23.422  1.00  24.40
     ATOM  3465  O   GLU A 455  0   -1.953  39.161  23.700  1.00  24.30
     ATOM  3466  CB  GLU A 455  0    0.399  38.090  21.830  1.00  27.20
     ATOM  3467  CG  GLU A 455  0    0.602  39.599  21.595  1.00  33.86
     ATOM  3468  CD  GLU A 455  0    1.783  40.205  22.309  1.00  37.49
20   ATOM  3469  OE1 GLU A 455  0    2.311  39.657  23.320  1.00  41.51
     ATOM  3470  OE2 GLU A 455  0    2.303  41.284  21.907  1.00  41.22
     ATOM  3471  N   PHE A 456  0   -2.347  37.005  23.334  1.00  23.97
     ATOM  3472  CA  PHE A 456  0   -3.775  37.163  23.516  1.00  24.68
     ATOM  3473  C   PHE A 456  0   -4.084  37.533  24.959  1.00  25.11
25   ATOM  3474  O   PHE A 456  0   -5.181  38.092  25.170  1.00  27.37
     ATOM  3475  CB  PHE A 456  0   -4.552  35.919  23.023  1.00  24.76
     ATOM  3476  CG  PHE A 456  0   -4.098  35.614  21.606  1.00  24.98
     ATOM  3477  CD1 PHE A 456  0   -4.392  36.500  20.590  1.00  24.98
     ATOM  3478  CD2 PHE A 456  0   -3.331  34.506  21.320  1.00  24.42
30   ATOM  3479  CE1 PHE A 456  0   -3.988  36.292  19.291  1.00  25.44
     ATOM  3480  CE2 PHE A 456  0   -2.913  34.293  20.015  1.00  26.40
     ATOM  3481  CZ  PHE A 456  0   -3.226  35.171  18.997  1.00  25.10
     ATOM  3482  N   HIS A 457  0   -3.205  37.294  25.922  1.00  22.35
     ATOM  3483  CA  HIS A 457  0   -3.508  37.682  27.291  1.00  22.55
35   ATOM  3484  C   HIS A 457  0   -3.053  39.121  27.561  1.00  23.81
     ATOM  3485  O   HIS A 457  0   -3.756  39.832  28.262  1.00  21.33
     ATOM  3486  CB  HIS A 457  0   -2.912  36.766  28.336  1.00  20.96
     ATOM  3487  CG  HIS A 457  0   -3.345  35.346  28.201  1.00  22.51
```

ATOM   3488 ND1 HIS A 457 0 -2.745 34.329 28.905 1.00 21.40
ATOM   3489 CD2 HIS A 457 0 -4.291 34.771 27.404 1.00 22.50
ATOM   3490 CE1 HIS A 457 0 -3.320 33.184 28.575 1.00 22.51
ATOM   3491 NE2 HIS A 457 0 -4.237 33.428 27.666 1.00 23.19
5 ATOM   3492 N   LEU A 458 0 -1.876 39.481 27.028 1.00 23.74
ATOM   3493 CA LEU A 458 0 -1.357 40.817 27.125 1.00 24.76
ATOM   3494 C   LEU A 458 0 -2.411 41.828 26.616 1.00 26.52
ATOM   3495 O   LEU A 458 0 -2.757 42.751 27.351 1.00 25.18
ATOM   3496 CB LEU A 458 0 -0.108 40.986 26.252 1.00 23.81
10 ATOM   3497 CG LEU A 458 0   0.898 42.062 26.624 1.00 24.09
ATOM   3498 CD1 LEU A 458 0   1.619 42.606 25.390 1.00 24.28
ATOM   3499 CD2 LEU A 458 0   0.351 43.195 27.462 1.00 23.72
ATOM   3500 N   MET A 459 0 -2.896 41.611 25.388 1.00 28.19
ATOM   3501 CA MET A 459 0 -3.914 42.458 24.785 1.00 31.98
15 ATOM   3502 C   MET A 459 0 -5.207 42.436 25.603 1.00 29.95
ATOM   3503 O   MET A 459 0 -5.886 43.439 25.520 1.00 29.10
ATOM   3504 CB MET A 459 0 -4.148 42.226 23.284 1.00 35.99
ATOM   3505 CG MET A 459 0 -5.056 41.103 22.852 1.00 42.66
ATOM   3506 SD MET A 459 0 -5.296 40.817 21.069 1.00 49.28
20 ATOM   3507 CE MET A 459 0 -6.238 39.291 21.119 1.00 47.39
ATOM   3508 N   ASN A 460 0 -5.523 41.486 26.464 1.00 29.07
ATOM   3509 CA ASN A 460 0 -6.706 41.539 27.296 1.00 29.41
ATOM   3510 C   ASN A 460 0 -6.407 41.908 28.746 1.00 28.46
ATOM   3511 O   ASN A 460 0 -7.183 41.577 29.645 1.00 26.89
25 ATOM   3512 CB ASN A 460 0 -7.537 40.253 27.210 1.00 31.34
ATOM   3513 CG ASN A 460 0 -8.325 40.243 25.900 1.00 33.82
ATOM   3514 OD1 ASN A 460 0 -7.909 39.609 24.926 1.00 34.29
ATOM   3515 ND2 ASN A 460 0 -9.437 40.971 25.861 1.00 34.55
ATOM   3516 N   GLY A 461 0 -5.320 42.655 28.981 1.00 26.30
30 ATOM   3517 CA GLY A 461 0 -5.020 43.198 30.268 1.00 24.99
ATOM   3518 C   GLY A 461 0 -4.043 42.601 31.235 1.00 24.75
ATOM   3519 O   GLY A 461 0 -3.879 43.228 32.304 1.00 22.69
ATOM   3520 N   LEU A 462 0 -3.375 41.478 30.914 1.00 22.85
ATOM   3521 CA LEU A 462 0 -2.478 40.872 31.913 1.00 22.10
35 ATOM   3522 C   LEU A 462 0 -1.071 41.485 31.890 1.00 21.56
ATOM   3523 O   LEU A 462 0 -0.116 40.876 31.415 1.00 20.28
ATOM   3524 CB LEU A 462 0 -2.477 39.376 31.669 1.00 20.03
ATOM   3525 CG LEU A 462 0 -2.010 38.393 32.720 1.00 20.40

```
   ATOM  3526 CD1 LEU A 462  0  -2.603 38.608 34.093 1.00 20.35
   ATOM  3527 CD2 LEU A 462  0  -2.385 36.983 32.229 1.00 21.01
   ATOM  3528 N   ALA A 463  0  -0.908 42.695 32.408 1.00 20.00
   ATOM  3529 CA  ALA A 463  0   0.350 43.432 32.381 1.00 20.74
 5 ATOM  3530 C   ALA A 463  0   0.398 44.511 33.481 1.00 21.85
   ATOM  3531 O   ALA A 463  0  -0.667 44.965 33.934 1.00 22.85
   ATOM  3532 CB  ALA A 463  0   0.559 44.179 31.060 1.00 15.13
   ATOM  3533 N   ILE A 464  0   1.605 44.810 33.950 1.00 19.91
   ATOM  3534 CA  ILE A 464  0   1.852 45.905 34.850 1.00 19.81
10 ATOM  3535 C   ILE A 464  0   3.180 46.579 34.434 1.00 19.41
   ATOM  3536 O   ILE A 464  0   3.938 46.003 33.660 1.00 18.24
   ATOM  3537 CB  ILE A 464  0   1.910 45.678 36.347 1.00 19.13
   ATOM  3538 CG1 ILE A 464  0   2.867 44.546 36.697 1.00 19.39
   ATOM  3539 CG2 ILE A 464  0   0.520 45.455 36.924 1.00 18.48
15 ATOM  3540 CD1 ILE A 464  0   3.205 44.549 38.179 1.00 21.00
   ATOM  3541 N   VAL A 465  0   3.380 47.791 34.924 1.00 18.95
   ATOM  3542 CA  VAL A 465  0   4.579 48.570 34.637 1.00 18.36
   ATOM  3543 C   VAL A 465  0   5.327 48.928 35.931 1.00 18.07
   ATOM  3544 O   VAL A 465  0   4.787 49.424 36.931 1.00 15.19
20 ATOM  3545 CB  VAL A 465  0   4.329 49.913 33.918 1.00 19.73
   ATOM  3546 CG1 VAL A 465  0   5.659 50.605 33.602 1.00 18.34
   ATOM  3547 CG2 VAL A 465  0   3.522 49.766 32.629 1.00 18.74
   ATOM  3548 N   PHE A 466  0   6.649 48.655 35.879 1.00 17.55
   ATOM  3549 CA  PHE A 466  0   7.499 49.051 37.013 1.00 14.72
25 ATOM  3550 C   PHE A 466  0   8.251 50.344 36.653 1.00 12.68
   ATOM  3551 O   PHE A 466  0   9.007 50.420 35.679 1.00 12.23
   ATOM  3552 CB  PHE A 466  0   8.484 47.978 37.381 1.00 15.19
   ATOM  3553 CG  PHE A 466  0   7.962 46.770 38.080 1.00 15.90
   ATOM  3554 CD1 PHE A 466  0   7.328 46.856 39.299 1.00 16.23
30 ATOM  3555 CD2 PHE A 466  0   8.153 45.533 37.492 1.00 16.23
   ATOM  3556 CE1 PHE A 466  0   6.861 45.720 39.936 1.00 15.97
   ATOM  3557 CE2 PHE A 466  0   7.665 44.389 38.133 1.00 18.27
   ATOM  3558 CZ  PHE A 466  0   7.018 44.480 39.352 1.00 16.74
   ATOM  3559 N   ALA A 467  0   8.045 51.361 37.443 1.00 10.60
35 ATOM  3560 CA  ALA A 467  0   8.788 52.648 37.194 1.00 12.27
   ATOM  3561 C   ALA A 467  0  10.007 52.526 38.111 1.00 12.02
   ATOM  3562 O   ALA A 467  0   9.905 52.728 39.325 1.00 12.43
   ATOM  3563 CB  ALA A 467  0   7.845 53.790 37.501 1.00 10.50
```

124

```
   ATOM  3564  N   GLU A 468  0   11.126  51.989  37.625  1.00 12.62
   ATOM  3565  CA  GLU A 468  0   12.263  51.683  38.515  1.00 14.63
   ATOM  3566  C   GLU A 468  0   13.195  52.883  38.685  1.00 13.91
   ATOM  3567  O   GLU A 468  0   13.631  53.369  37.651  1.00 13.05
 5 ATOM  3568  CB  GLU A 468  0   13.049  50.546  37.843  1.00 14.51
   ATOM  3569  CG  GLU A 468  0   14.256  50.035  38.629  1.00 16.84
   ATOM  3570  CD  GLU A 468  0   14.805  48.779  37.975  1.00 17.96
   ATOM  3571  OE1 GLU A 468  0   15.985  48.479  38.124  1.00 16.98
   ATOM  3572  OE2 GLU A 468  0   14.086  48.043  37.260  1.00 18.42
10 ATOM  3573  N   ASP A 469  0   13.546  53.286  39.886  1.00 15.17
   ATOM  3574  CA  ASP A 469  0   14.491  54.371  40.116  1.00 16.85
   ATOM  3575  C   ASP A 469  0   14.134  55.630  39.333  1.00 16.33
   ATOM  3576  O   ASP A 469  0   14.851  56.046  38.437  1.00 16.59
   ATOM  3577  CB  ASP A 469  0   15.899  53.920  39.748  1.00 19.86
15 ATOM  3578  CG  ASP A 469  0   17.040  54.766  40.289  1.00 21.40
   ATOM  3579  OD1 ASP A 469  0   16.811  55.793  40.943  1.00 22.21
   ATOM  3580  OD2 ASP A 469  0   18.216  54.403  40.069  1.00 22.21
   ATOM  3581  N   MET A 470  0   13.007  56.246  39.635  1.00 16.12
   ATOM  3582  CA  MET A 470  0   12.522  57.373  38.853  1.00 18.77
20 ATOM  3583  C   MET A 470  0   13.451  58.576  38.950  1.00 16.31
   ATOM  3584  O   MET A 470  0   13.591  59.208  37.925  1.00 13.55
   ATOM  3585  CB  MET A 470  0   11.116  57.847  39.302  1.00 20.06
   ATOM  3586  CG  MET A 470  0   10.041  56.941  38.684  1.00 23.99
   ATOM  3587  SD  MET A 470  0    8.375  57.337  39.283  1.00 26.08
25 ATOM  3588  CE  MET A 470  0    8.030  58.581  38.020  1.00 24.40
   ATOM  3589  N   ALA A 471  0   14.046  58.793  40.117  1.00 14.69
   ATOM  3590  CA  ALA A 471  0   14.953  59.906  40.287  1.00 16.97
   ATOM  3591  C   ALA A 471  0   16.141  59.864  39.335  1.00 18.79
   ATOM  3592  O   ALA A 471  0   16.602  60.956  38.945  1.00 21.08
30 ATOM  3593  CB  ALA A 471  0   15.471  59.927  41.728  1.00 17.62
   ATOM  3594  N   ASN A 472  0   16.623  58.695  38.912  1.00 17.28
   ATOM  3595  CA  ASN A 472  0   17.788  58.675  38.015  1.00 16.56
   ATOM  3596  C   ASN A 472  0   17.457  58.355  36.572  1.00 16.99
   ATOM  3597  O   ASN A 472  0   18.407  58.143  35.795  1.00 18.74
35 ATOM  3598  CB  ASN A 472  0   18.811  57.645  38.548  1.00 14.60
   ATOM  3599  CG  ASN A 472  0   19.417  58.132  39.887  1.00 14.00
   ATOM  3600  OD1 ASN A 472  0   18.895  57.830  40.967  1.00 12.71
   ATOM  3601  ND2 ASN A 472  0   20.468  58.916  39.775  1.00 10.80
```

```
   ATOM  3602 N   THR A 473  0  16.174 58.284 36.239 1.00 14.26
   ATOM  3603 CA  THR A 473  0  15.789 57.885 34.882 1.00 15.82
   ATOM  3604 C   THR A 473  0  16.150 58.891 33.812 1.00 16.81
   ATOM  3605 O   THR A 473  0  16.599 58.455 32.746 1.00 15.89
 5 ATOM  3606 CB  THR A 473  0  14.267 57.576 34.826 1.00 16.10
   ATOM  3607 OG1 THR A 473  0  14.001 56.416 35.609 1.00 15.41
   ATOM  3608 CG2 THR A 473  0  13.750 57.337 33.427 1.00 15.24
   ATOM  3609 N   VAL A 474  0  16.000 60.195 34.081 1.00 18.57
   ATOM  3610 CA  VAL A 474  0  16.355 61.192 33.050 1.00 21.06
10 ATOM  3611 C   VAL A 474  0  17.859 61.209 32.817 1.00 19.12
   ATOM  3612 O   VAL A 474  0  18.339 61.234 31.688 1.00 19.95
   ATOM  3613 CB  VAL A 474  0  15.860 62.616 33.424 1.00 22.91
   ATOM  3614 CG1 VAL A 474  0  16.467 63.702 32.538 1.00 23.06
   ATOM  3615 CG2 VAL A 474  0  14.346 62.721 33.334 1.00 23.04
15 ATOM  3616 N   ASP A 475  0  18.647 61.175 33.886 1.00 19.20
   ATOM  3617 CA  ASP A 475  0  20.109 61.168 33.741 1.00 18.98
   ATOM  3618 C   ASP A 475  0  20.578 59.899 33.047 1.00 17.52
   ATOM  3619 O   ASP A 475  0  21.386 60.028 32.130 1.00 18.31
   ATOM  3620 CB  ASP A 475  0  20.780 61.273 35.119 1.00 20.27
20 ATOM  3621 CG  ASP A 475  0  22.283 61.075 35.107 1.00 20.18
   ATOM  3622 OD1 ASP A 475  0  22.950 61.889 34.431 1.00 21.73
   ATOM  3623 OD2 ASP A 475  0  22.798 60.139 35.750 1.00 18.03
   ATOM  3624 N   ALA A 476  0  20.062 58.725 33.392 1.00 18.26
   ATOM  3625 CA  ALA A 476  0  20.539 57.486 32.793 1.00 18.93
25 ATOM  3626 C   ALA A 476  0  20.165 57.269 31.343 1.00 20.62
   ATOM  3627 O   ALA A 476  0  20.845 56.502 30.661 1.00 22.64
   ATOM  3628 CB  ALA A 476  0  19.966 56.298 33.551 1.00 18.48
   ATOM  3629 N   ASN A 477  0  19.047 57.787 30.858 1.00 22.66
   ATOM  3630 CA  ASN A 477  0  18.605 57.512 29.491 1.00 25.22
30 ATOM  3631 C   ASN A 477  0  18.578 58.782 28.683 1.00 28.55
   ATOM  3632 O   ASN A 477  0  17.969 59.755 29.143 1.00 30.20
   ATOM  3633 CB  ASN A 477  0  17.172 56.948 29.560 1.00 24.22
   ATOM  3634 CG  ASN A 477  0  17.114 55.666 30.380 1.00 23.73
   ATOM  3635 OD1 ASN A 477  0  16.747 55.672 31.570 1.00 21.33
35 ATOM  3636 ND2 ASN A 477  0  17.512 54.575 29.736 1.00 20.87
   ATOM  3637 N   ASN A 478  0  19.208 58.878 27.514 1.00 31.69
   ATOM  3638 CA  ASN A 478  0  19.036 60.131 26.776 1.00 33.61
   ATOM  3639 C   ASN A 478  0  18.758 59.770 25.331 1.00 32.22
```

```
   ATOM  3640 O   ASN A 478 0  19.602 59.478 24.508 1.00 32.16
   ATOM  3641 CB  ASN A 478 0  20.086 61.194 27.017 1.00 38.57
   ATOM  3642 CG  ASN A 478 0  21.426 60.602 27.370 1.00 40.94
   ATOM  3643 OD1 ASN A 478 0  21.928 59.903 26.484 1.00 44.60
 5 ATOM  3644 ND2 ASN A 478 0  21.866 60.861 28.578 1.00 41.32
   ATOM  3645 N   PRO A 479 0  17.461 59.733 25.075 1.00 32.37
   ATOM  3646 CA  PRO A 479 0  16.890 59.381 23.790 1.00 31.84
   ATOM  3647 C   PRO A 479 0  17.268 60.448 22.776 1.00 32.35
   ATOM  3648 O   PRO A 479 0  17.422 61.609 23.136 1.00 32.66
10 ATOM  3649 CB  PRO A 479 0  15.364 59.385 23.931 1.00 31.68
   ATOM  3650 CG  PRO A 479 0  15.126 59.724 25.373 1.00 31.69
   ATOM  3651 CD  PRO A 479 0  16.416 60.071 26.064 1.00 32.23
   ATOM  3652 N   PRO A 480 0  17.399 60.036 21.537 1.00 31.62
   ATOM  3653 CA  PRO A 480 0  17.670 60.939 20.422 1.00 30.72
15 ATOM  3654 C   PRO A 480 0  16.452 61.827 20.225 1.00 30.37
   ATOM  3655 O   PRO A 480 0  15.362 61.525 20.733 1.00 29.47
   ATOM  3656 CB  PRO A 480 0  17.935 60.035 19.203 1.00 29.87
   ATOM  3657 CG  PRO A 480 0  17.111 58.811 19.590 1.00 30.44
   ATOM  3658 CD  PRO A 480 0  17.161 58.657 21.093 1.00 30.35
20 ATOM  3659 N   VAL A 481 0  16.559 62.906 19.458 1.00 31.72
   ATOM  3660 CA  VAL A 481 0  15.398 63.788 19.268 1.00 30.68
   ATOM  3661 C   VAL A 481 0  14.335 63.090 18.446 1.00 29.51
   ATOM  3662 O   VAL A 481 0  13.134 63.284 18.648 1.00 27.97
   ATOM  3663 CB  VAL A 481 0  15.818 65.132 18.648 1.00 33.04
25 ATOM  3664 CG1 VAL A 481 0  16.126 65.010 17.161 1.00 31.91
   ATOM  3665 CG2 VAL A 481 0  14.717 66.171 18.907 1.00 33.32
   ATOM  3666 N   GLU A 482 0  14.746 62.167 17.562 1.00 28.90
   ATOM  3667 CA  GLU A 482 0  13.755 61.402 16.803 1.00 29.62
   ATOM  3668 C   GLU A 482 0  12.839 60.565 17.691 1.00 28.33
30 ATOM  3669 O   GLU A 482 0  11.704 60.287 17.280 1.00 28.36
   ATOM  3670 CB  GLU A 482 0  14.449 60.498 15.788 1.00 30.63
   ATOM  3671 CG  GLU A 482 0  15.143 61.256 14.666 1.00 32.78
   ATOM  3672 CD  GLU A 482 0  16.522 61.784 14.990 1.00 34.96
   ATOM  3673 OE1 GLU A 482 0  17.021 61.746 16.141 1.00 34.62
35 ATOM  3674 OE2 GLU A 482 0  17.170 62.297 14.033 1.00 37.13
   ATOM  3675 N   TRP A 483 0  13.311 60.124 18.857 1.00 25.91
   ATOM  3676 CA  TRP A 483 0  12.496 59.280 19.711 1.00 25.49
   ATOM  3677 C   TRP A 483 0  11.224 60.011 20.125 1.00 26.47
```

ATOM 3678 O   TRP A 483 0 10.155 59.405 20.116 1.00 26.95

ATOM 3679 CB TRP A 483 0 13.216 58.807 20.974 1.00 21.98

ATOM 3680 CG TRP A 483 0 12.376 58.144 22.013 1.00 21.49

ATOM 3681 CD1 TRP A 483 0 11.960 56.827 22.003 1.00 20.81

5 ATOM 3682 CD2 TRP A 483 0 11.818 58.730 23.194 1.00 20.14

ATOM 3683 NE1 TRP A 483 0 11.187 56.575 23.143 1.00 20.29

ATOM 3684 CE2 TRP A 483 0 11.097 57.736 23.868 1.00 20.29

ATOM 3685 CE3 TRP A 483 0 11.875 60.006 23.754 1.00 21.32

ATOM 3686 CZ2 TRP A 483 0 10.422 57.973 25.062 1.00 20.89

10 ATOM 3687 CZ3 TRP A 483 0 11.217 60.248 24.946 1.00 20.78

ATOM 3688 CH2 TRP A 483 0 10.495 59.227 25.596 1.00 21.44

ATOM 3689 N   ALA A 484 0 11.342 61.261 20.560 1.00 28.59

ATOM 3690 CA ALA A 484 0 10.165 62.003 21.029 1.00 30.73

ATOM 3691 C   ALA A 484 0   9.226 62.350 19.869 1.00 30.42

15 ATOM 3692 O   ALA A 484 0   8.024 62.337 20.071 1.00 31.34

ATOM 3693 CB ALA A 484 0 10.583 63.244 21.806 1.00 31.05

ATOM 3694 N   GLN A 485 0   9.702 62.488 18.653 1.00 30.79

ATOM 3695 CA GLN A 485 0   8.927 62.742 17.466 1.00 33.16

ATOM 3696 C   GLN A 485 0   8.026 61.608 17.017 1.00 32.81

20 ATOM 3697 O   GLN A 485 0   7.044 61.847 16.302 1.00 32.74

ATOM 3698 CB GLN A 485 0   9.859 63.113 16.290 1.00 34.56

ATOM 3699 CG GLN A 485 0 10.631 64.361 16.686 1.00 39.67

ATOM 3700 CD GLN A 485 0 11.559 64.919 15.640 1.00 42.86

ATOM 3701 OE1 GLN A 485 0 11.528 66.145 15.434 1.00 45.48

25 ATOM 3702 NE2 GLN A 485 0 12.375 64.103 14.982 1.00 44.07

ATOM 3703 N   LEU A 486 0   8.328 60.380 17.443 1.00 30.46

ATOM 3704 CA LEU A 486 0   7.500 59.231 17.095 1.00 27.76

ATOM 3705 C   LEU A 486 0   6.051 59.510 17.509 1.00 28.23

ATOM 3706 O   LEU A 486 0   5.100 59.331 16.752 1.00 26.71

30 ATOM 3707 CB LEU A 486 0   8.043 58.034 17.838 1.00 25.03

ATOM 3708 CG LEU A 486 0   8.988 57.012 17.226 1.00 24.18

ATOM 3709 CD1 LEU A 486 0   9.780 57.416 16.011 1.00 21.41

ATOM 3710 CD2 LEU A 486 0   9.864 56.464 18.342 1.00 23.28

ATOM 3711 N   CYS A 487 0   5.870 59.974 18.739 1.00 28.05

35 ATOM 3712 CA CYS A 487 0   4.560 60.263 19.279 1.00 30.77

ATOM 3713 C   CYS A 487 0   3.823 61.350 18.499 1.00 33.19

ATOM 3714 O   CYS A 487 0   2.627 61.170 18.263 1.00 33.69

ATOM 3715 CB CYS A 487 0   4.643 60.637 20.752 1.00 27.94

ATOM 3716 SG CYS A 487 0   5.214 59.280 21.781 1.00 27.23
ATOM 3717 N   GLU A 488 0   4.543 62.373 18.064 1.00 35.80
ATOM 3718 CA GLU A 488 0   3.871 63.458 17.334 1.00 39.12
ATOM 3719 C   GLU A 488 0   3.384 62.928 15.995 1.00 37.78
5 ATOM 3720 O   GLU A 488 0   2.186 63.025 15.711 1.00 37.61
ATOM 3721 CB GLU A 488 0   4.737 64.697 17.257 1.00 42.04
ATOM 3722 CG GLU A 488 0   5.667 64.822 16.064 1.00 47.75
ATOM 3723 CD GLU A 488 0   5.634 66.239 15.500 1.00 51.36
ATOM 3724 OE1 GLU A 488 0   5.501 66.422 14.266 1.00 52.66
10 ATOM 3725 OE2 GLU A 488 0   5.743 67.154 16.358 1.00 53.40
ATOM 3726 N   ILE A 489 0   4.263 62.253 15.267 1.00 36.63
ATOM 3727 CA ILE A 489 0   3.906 61.647 14.004 1.00 36.74
ATOM 3728 C   ILE A 489 0   2.754 60.662 14.113 1.00 36.98
ATOM 3729 O   ILE A 489 0   1.847 60.664 13.276 1.00 38.60
15 ATOM 3730 CB ILE A 489 0   5.089 60.903 13.361 1.00 36.57
ATOM 3731 CG1 ILE A 489 0   6.267 61.853 13.148 1.00 36.46
ATOM 3732 CG2 ILE A 489 0   4.651 60.305 12.030 1.00 36.90
ATOM 3733 CD1 ILE A 489 0   7.535 61.194 12.654 1.00 35.62
ATOM 3734 N   TYR A 490 0   2.758 59.808 15.105 1.00 36.22
20 ATOM 3735 CA TYR A 490 0   1.771 58.765 15.298 1.00 35.95
ATOM 3736 C   TYR A 490 0   0.413 59.314 15.692 1.00 37.83
ATOM 3737 O   TYR A 490 0 -0.581 58.816 15.165 1.00 39.24
ATOM 3738 CB TYR A 490 0   2.206 57.817 16.409 1.00 32.47
ATOM 3739 CG TYR A 490 0   1.314 56.641 16.663 1.00 30.55
25 ATOM 3740 CD1 TYR A 490 0   1.176 55.623 15.726 1.00 29.96
ATOM 3741 CD2 TYR A 490 0   0.610 56.536 17.849 1.00 29.79
ATOM 3742 CE1 TYR A 490 0   0.378 54.528 15.975 1.00 29.51
ATOM 3743 CE2 TYR A 490 0 -0.192 55.441 18.114 1.00 29.64
ATOM 3744 CZ TYR A 490 0 -0.288 54.445 17.171 1.00 29.51
30 ATOM 3745 OH TYR A 490 0 -1.101 53.363 17.437 1.00 32.06
ATOM 3746 N   ASP A 491 0   0.369 60.302 16.564 1.00 40.86
ATOM 3747 CA ASP A 491 0 -0.909 60.887 16.963 1.00 43.97
ATOM 3748 C   ASP A 491 0 -1.586 61.633 15.811 1.00 45.30
ATOM 3749 O   ASP A 491 0 -2.809 61.752 15.820 1.00 45.60
35 ATOM 3750 CB ASP A 491 0 -0.764 61.800 18.170 1.00 44.67
ATOM 3751 CG ASP A 491 0 -0.441 61.101 19.475 1.00 45.90
ATOM 3752 OD1 ASP A 491 0   0.149 61.761 20.364 1.00 46.32
ATOM 3753 OD2 ASP A 491 0 -0.763 59.911 19.669 1.00 46.04

ATOM 3754 N ASP A 492 0 -0.871 62.107 14.817 1.00 46.75
ATOM 3755 CA ASP A 492 0 -1.323 62.804 13.653 1.00 48.98
ATOM 3756 C ASP A 492 0 -1.702 61.936 12.460 1.00 49.48
ATOM 3757 O ASP A 492 0 -2.002 62.458 11.378 1.00 50.24
5 ATOM 3758 CB ASP A 492 0 -0.155 63.649 13.107 1.00 51.54
ATOM 3759 CG ASP A 492 0 -0.168 65.081 13.587 1.00 53.57
ATOM 3760 OD1 ASP A 492 0 -0.886 65.375 14.570 1.00 54.07
ATOM 3761 OD2 ASP A 492 0 0.576 65.857 12.939 1.00 55.04
ATOM 3762 N LEU A 493 0 -1.554 60.630 12.584 1.00 49.01
10 ATOM 3763 CA LEU A 493 0 -1.896 59.732 11.483 1.00 47.63
ATOM 3764 C LEU A 493 0 -3.377 59.872 11.137 1.00 47.61
ATOM 3765 O LEU A 493 0 -4.209 60.018 12.027 1.00 47.02
ATOM 3766 CB LEU A 493 0 -1.661 58.296 11.940 1.00 46.08
ATOM 3767 CG LEU A 493 0 -0.485 57.463 11.464 1.00 45.24
15 ATOM 3768 CD1 LEU A 493 0 0.616 58.224 10.756 1.00 43.57
ATOM 3769 CD2 LEU A 493 0 0.075 56.710 12.669 1.00 44.62
ATOM 3770 N PRO A 494 0 -3.694 59.763 9.866 1.00 48.01
ATOM 3771 CA PRO A 494 0 -5.049 59.734 9.353 1.00 49.11
ATOM 3772 C PRO A 494 0 -5.617 58.339 9.570 1.00 51.21
20 ATOM 3773 O PRO A 494 0 -4.919 57.325 9.495 1.00 50.61
ATOM 3774 CB PRO A 494 0 -4.938 59.995 7.843 1.00 48.94
ATOM 3775 CG PRO A 494 0 -3.559 59.463 7.544 1.00 48.47
ATOM 3776 CD PRO A 494 0 -2.714 59.538 8.797 1.00 48.22
ATOM 3777 N PRO A 495 0 -6.915 58.238 9.796 1.00 53.24
25 ATOM 3778 CA PRO A 495 0 -7.630 57.006 10.055 1.00 53.93
ATOM 3779 C PRO A 495 0 -7.404 55.890 9.058 1.00 54.84
ATOM 3780 O PRO A 495 0 -7.348 54.705 9.423 1.00 55.08
ATOM 3781 CB PRO A 495 0 -9.126 57.362 10.146 1.00 54.40
ATOM 3782 CG PRO A 495 0 -9.090 58.848 10.391 1.00 54.17
30 ATOM 3783 CD PRO A 495 0 -7.787 59.420 9.895 1.00 53.58
ATOM 3784 N GLU A 496 0 -7.190 56.198 7.784 1.00 55.36
ATOM 3785 CA GLU A 496 0 -6.936 55.187 6.763 1.00 55.83
ATOM 3786 C GLU A 496 0 -5.582 54.521 6.971 1.00 54.09
ATOM 3787 O GLU A 496 0 -5.345 53.406 6.505 1.00 53.29
35 ATOM 3788 CB GLU A 496 0 -7.091 55.805 5.378 1.00 57.96
ATOM 3789 CG GLU A 496 0 -6.030 55.604 4.339 1.00 61.30
ATOM 3790 CD GLU A 496 0 -6.448 54.984 3.025 1.00 63.68
ATOM 3791 OE1 GLU A 496 0 -7.449 55.411 2.388 1.00 65.15

ATOM 3792 OE2 GLU A 496 0 -5.747 54.034 2.586 1.00 64.91
ATOM 3793 N ALA A 497 0 -4.665 55.217 7.630 1.00 52.35
ATOM 3794 CA ALA A 497 0 -3.326 54.738 7.886 1.00 50.83
ATOM 3795 C ALA A 497 0 -3.245 53.626 8.924 1.00 49.08
5 ATOM 3796 O ALA A 497 0 -2.361 52.773 8.794 1.00 47.61
ATOM 3797 CB ALA A 497 0 -2.443 55.910 8.317 1.00 51.23
ATOM 3798 N THR A 498 0 -4.113 53.630 9.926 1.00 48.01
ATOM 3799 CA THR A 498 0 -4.086 52.617 10.964 1.00 48.73
ATOM 3800 C THR A 498 0 -5.271 51.656 10.938 1.00 48.99
10 ATOM 3801 O THR A 498 0 -5.425 50.852 11.862 1.00 47.81
ATOM 3802 CB THR A 498 0 -4.055 53.223 12.388 1.00 49.04
ATOM 3803 OG1 THR A 498 0 -5.315 53.816 12.752 1.00 47.95
ATOM 3804 CG2 THR A 498 0 -2.919 54.223 12.514 1.00 48.94
ATOM 3805 N SER A 499 0 -6.101 51.756 9.911 1.00 49.78
15 ATOM 3806 CA SER A 499 0 -7.307 50.933 9.814 1.00 51.20
ATOM 3807 C SER A 499 0 -7.048 49.470 9.494 1.00 49.98
ATOM 3808 O SER A 499 0 -6.257 49.143 8.617 1.00 48.80
ATOM 3809 CB SER A 499 0 -8.223 51.606 8.800 1.00 52.62
ATOM 3810 OG SER A 499 0 -8.428 50.827 7.596 1.00 55.22
20 ATOM 3811 N ILE A 500 0 -7.706 48.585 10.230 1.00 50.08
ATOM 3812 CA ILE A 500 0 -7.563 47.151 10.077 1.00 51.25
ATOM 3813 C ILE A 500 0 -8.642 46.518 9.207 1.00 53.08
ATOM 3814 O ILE A 500 0 -9.785 46.351 9.639 1.00 54.00
ATOM 3815 CB ILE A 500 0 -7.631 46.428 11.436 1.00 50.61
25 ATOM 3816 CG1 ILE A 500 0 -6.475 46.866 12.336 1.00 50.22
ATOM 3817 CG2 ILE A 500 0 -7.619 44.907 11.302 1.00 50.34
ATOM 3818 CD1 ILE A 500 0 -6.806 46.617 13.800 1.00 50.52
ATOM 3819 N GLN A 501 0 -8.263 46.074 8.024 1.00 54.35
ATOM 3820 CA GLN A 501 0 -9.177 45.360 7.129 1.00 55.14
30 ATOM 3821 C GLN A 501 0 -9.298 43.904 7.564 1.00 55.85
ATOM 3822 O GLN A 501 0 -8.335 43.130 7.556 1.00 55.59
ATOM 3823 CB GLN A 501 0 -8.594 45.485 5.732 1.00 55.56
ATOM 3824 CG GLN A 501 0 -9.262 44.736 4.604 1.00 56.32
ATOM 3825 CD GLN A 501 0 -8.874 45.369 3.271 1.00 57.46
35 ATOM 3826 OE1 GLN A 501 0 -8.480 44.667 2.336 1.00 57.35
ATOM 3827 NE2 GLN A 501 0 -8.998 46.697 3.219 1.00 57.61
ATOM 3828 N THR A 502 0 -10.493 43.506 7.968 1.00 57.08
ATOM 3829 CA THR A 502 0 -10.788 42.146 8.401 1.00 58.28

```
    ATOM  3830 C   THR A 502 0 -10.966 41.205  7.216 1.00 58.80
    ATOM  3831 O   THR A 502 0 -11.199 41.604  6.074 1.00 58.71
    ATOM  3832 CB  THR A 502 0 -12.046 42.108  9.293 1.00 58.99
    ATOM  3833 OG1 THR A 502 0 -11.794 42.909 10.464 1.00 59.62
  5 ATOM  3834 CG2 THR A 502 0 -12.421 40.707  9.749 1.00 58.74
    ATOM  3835 N   VAL A 503 0 -10.746 39.922  7.471 1.00 59.20
    ATOM  3836 CA  VAL A 503 0 -10.904 38.877  6.468 1.00 60.27
    ATOM  3837 C   VAL A 503 0 -11.687 37.736  7.119 1.00 61.11
    ATOM  3838 O   VAL A 503 0 -11.606 37.563  8.341 1.00 61.03
 10 ATOM  3839 CB  VAL A 503 0  -9.589 38.430  5.823 1.00 59.97
    ATOM  3840 CG1 VAL A 503 0  -8.337 38.964  6.507 1.00 59.65
    ATOM  3841 CG2 VAL A 503 0  -9.467 36.914  5.722 1.00 59.97
    ATOM  3842 N   VAL A 504 0 -12.478 37.002  6.341 1.00 61.77
    ATOM  3843 CA  VAL A 504 0 -13.203 35.863  6.911 1.00 62.40
 15 ATOM  3844 C   VAL A 504 0 -12.673 34.579  6.259 1.00 62.99
    ATOM  3845 O   VAL A 504 0 -11.811 33.894  6.803 1.00 63.13
    ATOM  3846 CB  VAL A 504 0 -14.730 35.882  6.756 1.00 62.39
    ATOM  3847 CG1 VAL A 504 0 -15.392 36.931  7.635 1.00 61.89
    ATOM  3848 CG2 VAL A 504 0 -15.127 36.068  5.297 1.00 62.17
 20 ATOM  3849 C1  NAG A 800 0  -2.401 42.835 45.802 1.00 30.44
    ATOM  3850 C2  NAG A 800 0  -1.327 43.232 46.780 1.00 31.80
    ATOM  3851 N2  NAG A 800 0  -0.119 43.561 45.983 1.00 31.37
    ATOM  3852 C7  NAG A 800 0   0.179 44.844 45.683 1.00 32.37
    ATOM  3853 O7  NAG A 800 0  -0.549 45.688 45.982 1.00 34.61
 25 ATOM  3854 C8  NAG A 800 0   1.457 45.094 44.983 1.00 31.67
    ATOM  3855 C3  NAG A 800 0  -1.015 42.187 47.801 1.00 32.94
    ATOM  3856 O3  NAG A 800 0  -0.264 42.838 48.796 1.00 34.46
    ATOM  3857 C4  NAG A 800 0  -2.351 41.662 48.377 1.00 34.05
    ATOM  3858 O4  NAG A 800 0  -2.097 40.644 49.344 1.00 35.62
 30 ATOM  3859 C5  NAG A 800 0  -3.128 41.025 47.202 1.00 35.11
    ATOM  3860 O5  NAG A 800 0  -3.466 42.046 46.295 1.00 33.06
    ATOM  3861 C6  NAG A 800 0  -4.444 40.420 47.673 1.00 36.66
    ATOM  3862 O6  NAG A 800 0  -5.199 41.411 48.288 1.00 39.73
    ATOM  3863 C1  GLC A 900 0  -8.957 50.280  6.333 1.00 58.53
 35 ATOM  3864 C2  GLC A 900 0  -8.500 49.605  5.037 1.00 59.25
    ATOM  3865 C3  GLC A 900 0  -7.806 50.686  4.219 1.00 59.71
    ATOM  3866 C4  GLC A 900 0  -8.691 51.905  3.987 1.00 60.13
    ATOM  3867 C5  GLC A 900 0  -9.595 52.289  5.142 1.00 59.22
```

```
   ATOM 3868 O5  GLC A 900 0 -10.004 51.177  5.937 1.00 59.71
   ATOM 3869 CU  IUM B  1 0  -1.332 34.401 30.132 1.00 29.47
   ATOM 3870 CU  IUM B  2 0   7.297 42.245 26.618 1.00 27.01
   ATOM 3871 CU  IUM B  3 0   9.569 38.786 23.923 1.00 21.38
 5 ATOM 3872 O   IUM B  5 0   7.445 40.703 25.162 1.00 26.99
   ATOM 3873 OW0 WAT W  1 0  19.509 36.893 30.054 1.00 13.07
   ATOM 3874 OW0 WAT W  2 0  24.726 29.672 16.651 1.00  7.67
   ATOM 3875 OW0 WAT W  3 0  15.295 17.988 35.061 1.00  8.65
   ATOM 3876 OW0 WAT W  4 0   6.481 28.311 23.427 1.00  8.00
10 ATOM 3877 OW0 WAT W  5 0  14.921 45.178 24.306 1.00 17.04
   ATOM 3878 OW0 WAT W  6 0  14.413 44.401 28.162 1.00 10.12
   ATOM 3879 OW0 WAT W  7 0   9.967 21.576  9.620 1.00 11.43
   ATOM 3880 OW0 WAT W  8 0  10.088 28.675 13.038 1.00  9.27
   ATOM 3881 OW0 WAT W  9 0   9.808 47.902 28.959 1.00 12.71
15 ATOM 3882 OW0 WAT W 10 0  21.976 23.052 35.604 1.00 11.72
   ATOM 3883 OW0 WAT W 11 0  10.862 25.744 29.928 1.00 10.21
   ATOM 3884 OW0 WAT W 12 0  26.087 32.996 23.097 1.00 14.21
   ATOM 3885 OW0 WAT W 13 0  22.256 58.745 37.931 1.00 17.85
   ATOM 3886 OW0 WAT W 14 0  -0.104 29.831 35.249 1.00 16.36
20 ATOM 3887 OW0 WAT W 15 0  18.153 61.857 36.641 1.00 14.38
   ATOM 3888 OW0 WAT W 16 0   9.426 38.431  9.161 1.00 15.35
   ATOM 3889 OW0 WAT W 17 0   7.639 24.371  3.713 1.00 22.18
   ATOM 3890 OW0 WAT W 18 0  27.977 11.643  9.481 1.00 19.22
   ATOM 3891 OW0 WAT W 19 0   3.140 21.028 24.695 1.00 11.12
25 ATOM 3892 OW0 WAT W 20 0   9.847 20.701 30.902 1.00 16.16
   ATOM 3893 OW0 WAT W 21 0  -1.517 29.009 43.180 1.00 27.18
   ATOM 3894 OW0 WAT W 22 0   3.497 29.138 26.088 1.00 17.22
   ATOM 3895 OW0 WAT W 23 0  20.614 32.765 40.433 1.00 17.63
   ATOM 3896 OW0 WAT W 24 0  19.098 51.778 39.452 1.00 22.33
30 ATOM 3897 OW0 WAT W 25 0   0.977 21.396  5.064 1.00 18.54
   ATOM 3898 OW0 WAT W 26 0   8.546 16.150 21.761 1.00 16.40
   ATOM 3899 OW0 WAT W 27 0   6.102 19.858 10.350 1.00 17.79
   ATOM 3900 OW0 WAT W 28 0  11.702 55.189 41.955 1.00 18.92
   ATOM 3901 OW0 WAT W 29 0   3.360 42.251 18.209 1.00 16.26
35 ATOM 3902 OW0 WAT W 30 0   6.232 14.672 22.473 1.00 24.49
   ATOM 3903 OW0 WAT W 31 0  16.729 26.542 39.731 1.00 15.28
   ATOM 3904 OW0 WAT W 32 0   2.834 30.640 40.601 1.00 18.11
   ATOM 3905 OW0 WAT W 33 0  21.893 42.837 27.884 1.00 15.08
```

```
     ATOM  3906 OW0 WAT W 34 0   1.581 28.193 27.914 1.00 17.77
     ATOM  3907 OW0 WAT W 35 0  -3.503 21.749 11.578 1.00 15.32
     ATOM  3908 OW0 WAT W 36 0   7.131 33.344 11.786 1.00 18.18
     ATOM  3909 OW0 WAT W 37 0  17.312 38.603 29.961 1.00 14.75
  5  ATOM  3910 OW0 WAT W 38 0  -6.705 40.723 39.909 1.00 23.49
     ATOM  3911 OW0 WAT W 39 0   9.010 31.121 11.736 1.00 19.99
     ATOM  3912 OW0 WAT W 40 0   9.376 28.353 33.076 1.00 16.22
     ATOM  3913 OW0 WAT W 41 0  30.104 29.895 20.857 1.00 25.77
     ATOM  3914 OW0 WAT W 42 0  -6.950 33.663 21.335 1.00 26.62
 10  ATOM  3915 OW0 WAT W 43 0   8.541 27.867 36.827 1.00 12.80
     ATOM  3916 OW0 WAT W 44 0   3.590 21.651 11.893 1.00 14.46
     ATOM  3917 OW0 WAT W 45 0  23.290 21.665 37.787 1.00 28.75
     ATOM  3918 OW0 WAT W 46 0  22.724 11.873 22.270 1.00 23.07
     ATOM  3919 OW0 WAT W 47 0  -1.090 42.001 12.877 1.00 19.33
 15  ATOM  3920 OW0 WAT W 48 0  14.091 27.298 40.583 1.00 18.51
     ATOM  3921 OW0 WAT W 49 0   2.336 52.026 29.983 1.00 25.66
     ATOM  3922 OW0 WAT W 50 0  15.475 14.450 22.853 1.00 20.37
     ATOM  3923 OW0 WAT W 51 0  25.945 26.568 40.287 1.00 24.49
     ATOM  3924 OW0 WAT W 52 0  19.545 41.598 35.087 1.00 20.70
 20  ATOM  3925 OW0 WAT W 53 0  -3.802 47.942  9.638 1.00 29.98
     ATOM  3926 OW0 WAT W 54 0  -7.478 41.160  9.585 1.00 24.26
     ATOM  3927 OW0 WAT W 55 0  -2.938 29.733 36.048 1.00 22.93
     ATOM  3928 OW0 WAT W 56 0  29.051 32.114 22.680 1.00 22.50
     ATOM  3929 OW0 WAT W 57 0   0.360 29.505  5.595 1.00 17.78
 25  ATOM  3930 OW0 WAT W 58 0   8.583 57.422 21.440 1.00 21.90
     ATOM  3931 OW0 WAT W 59 0  25.151 31.947 34.812 1.00 22.13
     ATOM  3932 OW0 WAT W 60 0  25.133 62.204 32.968 1.00 25.75
     ATOM  3933 OW0 WAT W 61 0  14.909 40.770 30.294 1.00 17.25
     ATOM  3934 OW0 WAT W 62 0  20.825 30.520 34.676 1.00 16.18
 30  ATOM  3935 OW0 WAT W 63 0   5.509 26.744 43.167 1.00 30.12
     ATOM  3936 OW0 WAT W 64 0   5.280 57.279 14.627 1.00 22.66
     ATOM  3937 OW0 WAT W 65 0   2.944 53.436 32.359 1.00 22.97
     ATOM  3938 OW0 WAT W 66 0  11.266 43.508  3.407 1.00 20.01
     ATOM  3939 OW0 WAT W 67 0  21.535 45.549 26.563 1.00 24.47
 35  ATOM  3940 OW0 WAT W 68 0   0.412 33.358 11.837 1.00 19.89
     ATOM  3941 OW0 WAT W 69 0  26.466 32.305 25.785 1.00 20.19
     ATOM  3942 OW0 WAT W 70 0   0.910 45.068  7.829 1.00 22.05
     ATOM  3943 OW0 WAT W 71 0  -2.060 46.506 39.381 1.00 23.49
```

ATOM 3944 OW0 WAT W 72 0 20.236 56.718 25.851 1.00 23.74
ATOM 3945 OW0 WAT W 73 0 3.253 23.017 38.254 1.00 24.83
ATOM 3946 OW0 WAT W 74 0 9.653 22.835 35.143 1.00 25.79
ATOM 3947 OW0 WAT W 75 0 16.877 52.904 47.331 1.00 24.42
5 ATOM 3948 OW0 WAT W 76 0 14.293 22.021 3.993 1.00 32.28
ATOM 3949 OW0 WAT W 77 0 -5.287 19.835 18.528 1.00 24.65
ATOM 3950 OW0 WAT W 78 0 8.414 38.317 49.069 1.00 28.77
ATOM 3951 OW0 WAT W 79 0 7.070 32.466 47.926 1.00 21.83
ATOM 3952 OW0 WAT W 80 0 -0.452 28.307 25.779 1.00 16.58
10 ATOM 3953 OW0 WAT W 81 0 14.774 15.006 34.455 1.00 25.63
ATOM 3954 OW0 WAT W 82 0 11.515 54.942 35.962 1.00 14.20
ATOM 3955 OW0 WAT W 83 0 25.643 33.451 32.105 1.00 30.31
ATOM 3956 OW0 WAT W 84 0 11.869 12.221 20.394 1.00 31.37
ATOM 3957 OW0 WAT W 85 0 11.653 51.587 22.411 1.00 16.48
15 ATOM 3958 OW0 WAT W 86 0 17.334 40.837 51.079 1.00 30.26
ATOM 3959 OW0 WAT W 87 0 4.355 25.208 34.030 1.00 32.26
ATOM 3960 OW0 WAT W 88 0 18.816 52.360 32.512 1.00 21.19
ATOM 3961 OW0 WAT W 89 0 -2.704 46.518 35.364 1.00 21.99
ATOM 3962 OW0 WAT W 90 0 18.793 27.893 49.481 1.00 24.52
20 ATOM 3963 OW0 WAT W 91 0 22.459 46.584 28.898 1.00 18.99
ATOM 3964 OW0 WAT W 92 0 7.958 34.422 49.370 1.00 26.14
ATOM 3965 OW0 WAT W 93 0 23.972 16.246 6.806 1.00 24.35
ATOM 3966 OW0 WAT W 94 0 1.340 49.185 26.307 1.00 31.64
ATOM 3967 OW0 WAT W 95 0 -1.830 35.291 12.266 1.00 27.28
25 ATOM 3968 OW0 WAT W 96 0 20.460 17.486 3.589 1.00 33.51
ATOM 3969 OW0 WAT W 97 0 15.177 6.964 9.868 1.00 24.40
ATOM 3970 OW0 WAT W 98 0 18.616 57.927 43.922 1.00 30.76
ATOM 3971 OW0 WAT W 99 0 10.562 32.112 9.972 1.00 28.90
ATOM 3972 OW0 WAT W 100 0 1.630 61.363 10.878 1.00 33.92
30 ATOM 3973 OW0 WAT W 101 0 -4.939 49.989 33.211 1.00 29.73
ATOM 3974 OW0 WAT W 102 0 19.385 44.813 34.546 1.00 23.52
ATOM 3975 OW0 WAT W 103 0 19.055 43.063 37.581 1.00 30.59
ATOM 3976 OW0 WAT W 105 0 28.703 33.555 27.406 1.00 32.92
ATOM 3977 OW0 WAT W 106 0 28.835 19.646 10.759 1.00 40.44
35 ATOM 3978 OW0 WAT W 107 0 22.047 22.465 9.758 1.00 29.98
ATOM 3979 OW0 WAT W 108 0 14.689 61.032 36.346 1.00 30.63
ATOM 3980 OW0 WAT W 109 0 16.998 24.042 9.318 1.00 23.90
ATOM 3981 OW0 WAT W 110 0 13.472 30.533 11.848 1.00 34.83

```
   ATOM 3982 OW0 WAT W 111 0  -2.175 35.601 41.496 1.00 28.55
   ATOM 3983 OW0 WAT W 112 0   1.528 17.373 -1.396 1.00 38.21
   ATOM 3984 OW0 WAT W 113 0  -2.856 29.748 19.681 1.00 30.55
   ATOM 3985 OW0 WAT W 114 0   2.377 42.810 47.971 1.00 26.87
 5 ATOM 3986 OW0 WAT W 115 0  10.947 12.820 33.745 1.00 31.60
   ATOM 3987 OW0 WAT W 116 0   9.807 58.194 12.442 1.00 29.63
   ATOM 3988 OW0 WAT W 117 0  18.488 62.559 29.470 1.00 45.83
   ATOM 3989 OW0 WAT W 118 0  11.708 61.566 40.940 1.00 37.19
   ATOM 3990 OW0 WAT W 119 0 -10.101 22.257 15.091 1.00 30.48
10 ATOM 3991 OW0 WAT W 120 0  -1.930 15.913  7.386 1.00 36.63
   ATOM 3992 OW0 WAT W 121 0  23.988 43.686 29.319 1.00 32.15
   ATOM 3993 OW0 WAT W 122 0   7.354 57.153 12.809 1.00 28.10
   ATOM 3994 OW0 WAT W 123 0  24.207 22.101 11.958 1.00 32.83
   ATOM 3995 OW0 WAT W 124 0  -1.268 15.083  9.738 1.00 32.53
15 ATOM 3996 OW0 WAT W 125 0  19.363  5.047 13.812 1.00 34.57
   ATOM 3997 OW0 WAT W 126 0   4.799 41.145 23.688 1.00 28.33
   ATOM 3998 OW0 WAT W 127 0  15.975 23.287  5.889 1.00 30.95
   ATOM 3999 OW0 WAT W 128 0   3.698 38.582 -2.369 1.00 36.84
   ATOM 4000 OW0 WAT W 129 0  -2.601 49.124 11.710 1.00 28.91
20 ATOM 4001 OW0 WAT W 130 0  15.779 56.598 43.285 1.00 27.76
   ATOM 4002 OW0 WAT W 131 0  26.306 32.724 13.233 1.00 37.94
   ATOM 4003 OW0 WAT W 132 0   3.610 46.947 23.991 1.00 35.49
   ATOM 4004 OW0 WAT W 133 0  18.354 11.929 29.348 1.00 33.88
   ATOM 4005 OW0 WAT W 134 0  13.966 41.517 27.765 1.00 18.02
25 ATOM 4006 OW0 WAT W 135 0  23.545 49.080 27.785 1.00 25.21
   ATOM 4007 OW0 WAT W 136 0  16.876 25.082 41.791 1.00 28.71
   ATOM 4008 OW0 WAT W 137 0  15.439 54.809 45.527 1.00 35.30
   ATOM 4009 OW0 WAT W 138 0  11.733 25.676 43.264 1.00 38.24
   ATOM 4010 OW0 WAT W 139 0   9.795 34.460 11.898 1.00 31.61
30 ATOM 4011 OW0 WAT W 140 0  13.328 57.569 42.356 1.00 30.66
   ATOM 4012 OW0 WAT W 141 0  14.146  7.869 20.604 1.00 35.72
   ATOM 4013 OW0 WAT W 142 0  23.330 12.948  3.922 1.00 29.83
   ATOM 4014 OW0 WAT W 143 0  16.607 10.575 24.347 1.00 36.47
   ATOM 4015 OW0 WAT W 144 0   8.509 25.546 35.012 1.00 35.43
35 ATOM 4016 OW0 WAT W 145 0  12.597 44.457  1.450 1.00 39.54
   ATOM 4017 OW0 WAT W 146 0  21.680 51.509 39.154 1.00 40.08
   ATOM 4018 OW0 WAT W 147 0  -0.702 52.593 39.700 1.00 29.62
   ATOM 4019 OW0 WAT W 148 0  23.269 14.719 22.589 1.00 30.24
```

```
   ATOM  4020 OW0 WAT W 149 0  27.149 22.972 41.846 1.00 35.00
   ATOM  4021 OW0 WAT W 150 0   2.854  9.792  8.923 1.00 46.35
   ATOM  4022 OW0 WAT W 151 0  24.831 15.672 24.889 1.00 29.22
   ATOM  4023 OW0 WAT W 152 0  24.965 51.606 19.113 1.00 32.19
 5 ATOM  4024 OW0 WAT W 153 0  -4.611 25.034 37.817 1.00 46.51
   ATOM  4025 OW0 WAT W 154 0  12.225 39.382 28.864 1.00 25.42
   ATOM  4026 OW0 WAT W 155 0  18.332 22.341 43.180 1.00 36.18
   ATOM  4027 OW0 WAT W 156 0  36.467 20.701 17.144 1.00 44.13
   ATOM  4028 OW0 WAT W 157 0  -4.903 47.901 40.886 1.00 33.97
10 ATOM  4029 OW0 WAT W 158 0  12.979 13.955  3.208 1.00 33.60
   ATOM  4030 OW0 WAT W 159 0  32.383 12.693 24.743 1.00 30.25
   ATOM  4031 OW0 WAT W 160 0  30.796 26.296 14.368 1.00 44.37
   ATOM  4032 OW0 WAT W 161 0  19.332 37.280 40.057 1.00 31.54
   ATOM  4033 OW0 WAT W 162 0  17.625 20.028 41.642 1.00 45.88
15 ATOM  4034 OW0 WAT W 163 0  19.917 56.115 46.103 1.00 40.37
   ATOM  4035 OW0 WAT W 164 0  -4.743 14.204 16.748 1.00 40.86
   ATOM  4036 OW0 WAT W 165 0   0.738 46.912 21.790 1.00 38.56
   ATOM  4037 OW0 WAT W 166 0  22.648 62.277 30.976 1.00 24.37
   ATOM  4038 OW0 WAT W 167 0  -4.322 45.754 26.894 1.00 48.97
20 ATOM  4039 OW0 WAT W 168 0  -2.386 24.601  0.665 1.00 32.57
   ATOM  4040 OW0 WAT W 169 0  -0.459 41.618 35.838 1.00 35.25
   ATOM  4041 OW0 WAT W 170 0  26.659  4.722 11.434 1.00 41.25
   ATOM  4042 OW0 WAT W 171 0  13.720 11.379 22.121 1.00 39.59
   ATOM  4043 OW0 WAT W 172 0  15.266  7.451  6.576 1.00 41.71
25 ATOM  4044 OW0 WAT W 173 0   0.134 17.450  6.165 1.00 42.12
   ATOM  4045 OW0 WAT W 174 0  38.646 32.884 25.247 1.00 41.80
   ATOM  4046 OW0 WAT W 175 0  10.591 17.398  3.251 1.00 29.37
   ATOM  4047 OW0 WAT W 176 0  22.444 49.424 25.264 1.00 19.51
   ATOM  4048 OW0 WAT W 177 0   0.429 23.224 28.598 1.00 33.54
30 ATOM  4049 OW0 WAT W 178 0  -2.302 27.278 34.780 1.00 44.76
   ATOM  4050 OW0 WAT W 179 0   2.054 25.866 16.462 1.00 34.29
   ATOM  4051 OW0 WAT W 180 0  30.277 18.006 25.789 1.00 42.28
   ATOM  4052 OW0 WAT W 181 0   2.316 18.424 27.884 1.00 47.39
   ATOM  4053 OW0 WAT W 182 0  19.401 41.164 39.560 1.00 39.68
35 ATOM  4054 OW0 WAT W 183 0  23.742 10.982 24.879 1.00 43.32
   ATOM  4055 OW0 WAT W 184 0   3.926 24.450 44.251 1.00 48.95
   ATOM  4056 OW0 WAT W 185 0  25.186 21.211 40.951 1.00 39.05
   ATOM  4057 OW0 WAT W 186 0  20.353 34.816 48.799 1.00 34.08
```

```
   ATOM  4058 OW0 WAT W 187 0  35.782 22.476 21.693 1.00 40.04
   ATOM  4059 OW0 WAT W 188 0  27.256 23.617 12.235 1.00 40.85
   ATOM  4060 OW0 WAT W 189 0   6.777 12.502 12.641 1.00 53.37
   ATOM  4061 OW0 WAT W 190 0  -4.663 38.998  4.159 1.00 39.85
 5 ATOM  4062 OW0 WAT W 191 0  24.398 52.064 24.607 1.00 45.51
   ATOM  4063 OW0 WAT W 192 0   1.808 15.541  4.832 1.00 41.06
   ATOM  4064 OW0 WAT W 193 0   5.341 36.359  7.569 1.00 39.36
   ATOM  4065 OW0 WAT W 194 0  32.192 38.650 21.799 1.00 37.18
   ATOM  4066 OW0 WAT W 195 0 -10.782 36.616 38.705 1.00 50.35
10 ATOM  4067 OW0 WAT W 196 0   4.119 64.116 32.946 1.00 34.51
   ATOM  4068 OW0 WAT W 197 0  19.427 22.772  5.898 1.00 37.94
   ATOM  4069 OW0 WAT W 198 0  -4.671 33.476  1.652 1.00 43.38
   ATOM  4070 OW0 WAT W 199 0  -8.983 23.757 17.693 1.00 57.10
   ATOM  4071 OW0 WAT W 200 0  -6.735 22.473 20.432 1.00 38.49
15 ATOM  4072 OW0 WAT W 201 0  -6.954 26.746 37.309 1.00 55.48
   ATOM  4073 OW0 WAT W 202 0  23.418 38.662 33.700 1.00 42.20
   ATOM  4074 OW0 WAT W 203 0   9.004 24.070 36.971 1.00 40.06
   ATOM  4075 OW0 WAT W 204 0  18.890 42.920 51.502 1.00 46.29
   ATOM  4076 OW0 WAT W 205 0  13.301 18.514  3.624 1.00 42.17
20 ATOM  4077 OW0 WAT W 206 0  31.189 12.995 19.645 1.00 51.92
   ATOM  4078 OW0 WAT W 207 0  15.589 57.456 13.738 1.00 38.96
   ATOM  4079 OW0 WAT W 208 0  -3.389 12.961 12.738 1.00 46.99
   ATOM  4080 OW0 WAT W 209 0   9.321 30.475  6.320 1.00 49.75
   ATOM  4081 OW0 WAT W 210 0   1.680 61.379 33.738 1.00 37.48
25 ATOM  4082 OW0 WAT W 211 0  -3.811 36.417  3.807 1.00 46.01
   ATOM  4083 OW0 WAT W 212 0  17.087 46.902  3.830 1.00 45.12
   ATOM  4084 OW0 WAT W 213 0  23.702 22.325 43.022 1.00 36.14
   ATOM  4085 OW0 WAT W 214 0  10.849 60.003 14.389 1.00 32.05
   ATOM  4086 OW0 WAT W 215 0  34.001 25.493 20.855 1.00 40.75
30 ATOM  4087 OW0 WAT W 216 0  27.422 37.093 28.951 1.00 42.33
   ATOM  4088 OW0 WAT W 217 0   2.471 63.256 35.173 1.00 48.36
   ATOM  4089 OW0 WAT W 218 0  -0.973 59.086 28.720 1.00 53.14
   ATOM  4090 OW0 WAT W 219 0  28.841  9.287  6.463 1.00 39.02
   ATOM  4091 OW0 WAT W 220 0  -5.593 21.802  9.619 1.00 44.21
35 ATOM  4092 OW0 WAT W 221 0  22.109 15.521  1.696 1.00 38.33
   ATOM  4093 OW0 WAT W 222 0  13.029 32.860 12.233 1.00 37.63
   ATOM  4094 OW0 WAT W 223 0  11.840 33.823  3.800 1.00 42.20
   ATOM  4095 OW0 WAT W 224 0   8.476 42.976 -0.104 1.00 40.23
```

```
    ATOM  4096  OW0 WAT W 225 0    6.607   9.754 13.906  1.00 41.30
    ATOM  4097  OW0 WAT W 226 0   22.513  32.613 49.067  1.00 47.26
    ATOM  4098  OW0 WAT W 227 0   13.790   4.924 16.718  1.00 38.05
    ATOM  4099  OW0 WAT W 228 0    4.578  46.381  2.146  1.00 38.90
  5 ATOM  4100  OW0 WAT W 229 0   -0.178  18.054 23.533  1.00 43.42
    ATOM  4101  OW0 WAT W 230 0   -5.146  34.010  4.766  1.00 38.90
    ATOM  4102  OW0 WAT W 231 0   20.232  28.890 51.507  1.00 44.95
    ATOM  4103  OW0 WAT W 232 0   16.083  32.879 10.309  1.00 45.29
    ATOM  4104  OW0 WAT W 233 0   22.111  51.333 10.599  1.00 34.03
 10 ATOM  4105  OW0 WAT W 234 0    3.247  15.790 28.046  1.00 50.25
    ATOM  4106  OW0 WAT W 235 0    5.547  11.598  9.674  1.00 56.39
    ATOM  4107  OW0 WAT W 236 0   -1.085  18.297 -2.265  1.00 45.26
    ATOM  4108  OW0 WAT W 237 0   30.994  12.013 22.690  1.00 50.37
    ATOM  4109  OW0 WAT W 238 0   24.691  33.260 27.819  1.00 37.65
 15 ATOM  4110  OW0 WAT W 239 0   18.911  40.770  5.815  1.00 44.15
    ATOM  4111  OW0 WAT W 240 0   21.532  53.033 33.280  1.00 31.23
    ATOM  4112  OW0 WAT W 241 0   19.745  46.029  4.364  1.00 46.38
    ATOM  4113  OW0 WAT W 242 0   27.516  16.526 25.474  1.00 51.75
    ATOM  4114  OW0 WAT W 243 0   34.171  19.604  8.423  1.00 55.79
 20 ATOM  4115  OW0 WAT W 244 0   23.870  53.512 11.474  1.00 42.01
    ATOM  4116  OW0 WAT W 245 0   14.492  23.842 44.882  1.00 52.25
    ATOM  4117  OW0 WAT W 246 0   -3.070  63.260 33.189  1.00 40.77
    ATOM  4118  OW0 WAT W 247 0   22.185  55.701 37.353  1.00 39.52
    ATOM  4119  OW0 WAT W 248 0   14.144  26.239 42.825  1.00 42.50
 25 ATOM  4120  OW0 WAT W 249 0   25.026  36.545 35.213  1.00 58.19
    ATOM  4121  OW0 WAT W 250 0   27.072  34.293 43.895  1.00 46.58
    ATOM  4122  OW0 WAT W 251 0   11.742   7.192  4.856  1.00 42.78
    ATOM  4123  OW0 WAT W 252 0    0.730  46.405 24.947  1.00 39.31
    ATOM  4124  OW0 WAT W 253 0   28.346  34.036 30.808  1.00 43.10
 30 ATOM  4125  OW0 WAT W 254 0   -3.838  40.281  1.903  1.00 38.67
    ATOM  4126  OW0 WAT W 255 0    6.837  35.163 51.935  1.00 58.57
    ATOM  4127  OW0 WAT W 256 0   19.740  62.853 17.880  1.00 52.39
    ATOM  4128  OW0 WAT W 258 0   -0.994  41.755 22.088  0.00 69.57
    ATOM  4129  OW0 WAT W 259 0    1.221  10.473 15.458  1.00 54.80
 35 ATOM  4130  OW0 WAT W 260 0   23.445  55.367 31.430  1.00 48.90
    ATOM  4131  OW0 WAT W 261 0   23.757  57.854 34.657  1.00 37.69
    ATOM  4132  OW0 WAT W 262 0    8.508  19.111 34.572  1.00 55.52
    ATOM  4133  OW0 WAT W 263 0   22.806  22.381  3.611  1.00 64.20
```

```
   ATOM  4134  OW0 WAT W 264  0   0.398 22.602 42.625  1.00 58.86
   ATOM  4135  OW0 WAT W 265  0   4.195 52.287 43.465  1.00 36.84
   ATOM  4136  OW0 WAT W 266  0  20.211  6.536  4.911  1.00 39.34
   ATOM  4137  OW0 WAT W 267  0  14.680 16.117  2.803  1.00 45.76
 5 ATOM  4138  OW0 WAT W 268  0  14.938 25.582  6.850  1.00 41.01
   ATOM  4139  OW0 WAT W 269  0   7.763  7.940 31.891  0.00 71.30
   ATOM  4140  OW0 WAT W 270  0  -3.459 33.491 39.400  1.00 40.80
   ATOM  4141  OW0 WAT W 271  0  23.154 22.897  6.985  1.00 48.25
   ATOM  4142  OW0 WAT W 272  0  34.916 25.555 28.092  1.00 52.63
10 ATOM  4143  OW0 WAT W 273  0   8.332 45.481 50.776  1.00 47.23
   ATOM  4144  OW0 WAT W 274  0  -3.441 57.643 28.775  1.00 49.70
   ATOM  4145  OW0 WAT W 275  0  23.213 40.573 47.561  1.00 56.02
   ATOM  4146  OW0 WAT W 276  0   5.421 55.179 45.172  1.00 52.70
   ATOM  4147  OW0 WAT W 277  0  -3.012 21.908 40.933  1.00 41.69
15 ATOM  4148  OW0 WAT W 278  0  26.328 53.637 17.905  1.00 37.80
   ATOM  4149  OW0 WAT W 279  0   9.740 58.922 43.485  1.00 52.06
   ATOM  4150  OW0 WAT W 280  0  23.545 15.660  4.258  1.00 41.55
   ATOM  4151  OW0 WAT W 281  0  22.652 31.154 51.246  1.00 58.65
   ATOM  4152  OW0 WAT W 282  0  22.192 51.135  8.251  1.00 44.76
20 ATOM  4153  OW0 WAT W 283  0  -6.046 22.886 24.288  1.00 52.40
   ATOM  4154  OW0 WAT W 284  0  19.949 45.276 49.516  1.00 54.58
   ATOM  4155  OW0 WAT W 285  0   7.388 22.308 32.108  1.00 43.62
   ATOM  4156  OW0 WAT W 286  0  15.080 50.452  2.795  1.00 52.20
   ATOM  4157  OW0 WAT W 287  0   1.016 62.235 30.878  1.00 56.81
25 ATOM  4158  OW0 WAT W 288  0  23.803 52.570 27.699  1.00 56.22
   ATOM  4159  OW0 WAT W 289  0 -10.525 31.623 13.870  1.00 47.21
   ATOM  4160  OW0 WAT W 290  0   1.599 55.502 24.567  1.00 44.50
   ATOM  4161  OW0 WAT W 291  0 -15.671 37.251 14.660  1.00 83.62
   ATOM  4162  OW0 WAT W 292  0   7.231  7.950 17.754  1.00 50.61
30 ATOM  4163  OW0 WAT W 293  0  -4.009 34.057 42.492  1.00 78.48
   ATOM  4164  OW0 WAT W 294  0  21.004 58.371 18.690  1.00 61.15
   ATOM  4165  OW0 WAT W 295  0  16.405 48.869 52.211  1.00 53.17
   ATOM  4166  OW0 WAT W 296  0   7.329 31.202  1.964  1.00 38.86
   ATOM  4167  OW0 WAT W 297  0   9.518 53.886  5.467  1.00 41.62
35 ATOM  4168  OW0 WAT W 298  0  10.398 48.995  0.335  1.00 49.64
   ATOM  4169  OW0 WAT W 299  0   9.889 15.077  3.774  1.00 42.28
   ATOM  4170  OW0 WAT W 300  0  15.854 56.731 10.934  1.00 44.02
```

SEQUENCE LISTING

(1) GENERAL INFORMATION:

    (i) APPLICANT:
        (A) NAME: NOVO NORDISK
        (B) STREET: Novo Alle
        (C) CITY: Bagsvaerd
        (E) COUNTRY: Denmark
        (F) POSTAL CODE (ZIP): DK-2800
        (G) TELEPHONE: +45 44 44 88 88
        (H) TELEFAX: +45 44 49 05 55

    (ii) TITLE OF INVENTION: LACCASE MUTANTS

    (iii) NUMBER OF SEQUENCES: 10

    (iv) COMPUTER READABLE FORM:
        (A) MEDIUM TYPE: Floppy disk
        (B) COMPUTER: IBM PC compatible
        (C) OPERATING SYSTEM: PC-DOS/MS-DOS
        (D) SOFTWARE: PatentIn Release #1.0, Version #1.30 (EPO)

(2) INFORMATION FOR SEQ ID NO: 1:

    (i) SEQUENCE CHARACTERISTICS:
        (A) LENGTH: 539 amino acids
        (B) TYPE: amino acid
        (C) STRANDEDNESS: single
        (D) TOPOLOGY: linear

    (ii) MOLECULE TYPE: protein

    (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 1:

```
Met Phe Lys Asn Leu Leu Ser Phe Ala Leu Leu Ala Ile Ser Val Ala
1               5                   10                  15

Asn Ala Gln Ile Val Asn Ser Val Asp Thr Met Thr Leu Thr Asn Ala
            20                  25                  30

Asn Val Ser Pro Asp Gly Phe Thr Arg Ala Gly Ile Leu Val Asn Gly
            35                  40                  45

Val His Gly Pro Leu Ile Arg Gly Gly Lys Asn Asp Asn Phe Glu Leu
    50                  55                  60

Asn Val Val Asn Asp Leu Asp Asn Pro Thr Met Leu Arg Pro Thr Ser
65                  70                  75                  80

Ile His Trp His Gly Leu Phe Gln Arg Gly Thr Asn Trp Ala Asp Gly
                85                  90                  95

Ala Asp Gly Val Asn Gln Cys Pro Ile Ser Pro Gly His Ala Phe Leu
                100                 105                 110

Tyr Lys Phe Thr Pro Ala Gly His Ala Gly Thr Phe Trp Tyr His Ser
            115                 120                 125

His Phe Gly Thr Gln Tyr Cys Asp Gly Leu Arg Gly Pro Met Val Ile
            130                 135                 140

Tyr Asp Asp Asn Asp Pro His Ala Ala Leu Tyr Asp Glu Asp Asp Glu
145                 150                 155                 160
Asn Thr Ile Ile Thr Leu Ala Asp Trp Tyr His Ile Pro Ala Pro Ser
```

```
                           165                    170                    175
        Ile Gln Gly Ala Ala Gln Pro Asp Ala Thr Leu Ile Asn Gly Lys Gly
                     180                185                190
   5
        Arg Tyr Val Gly Gly Pro Ala Ala Glu Leu Ser Ile Val Asn Val Glu
                     195                200                205
        Gln Gly Lys Lys Tyr Arg Met Arg Leu Ile Ser Leu Ser Cys Asp Pro
  10         210                215                220
        Asn Trp Gln Phe Ser Ile Asp Gly His Glu Leu Thr Ile Ile Glu Val
        225                230                235                240
  15    Asp Gly Gln Leu Thr Glu Pro His Thr Val Asp Arg Leu Gln Ile Phe
                     245                250                255
        Thr Gly Gln Arg Tyr Ser Phe Val Leu Asp Ala Asn Gln Pro Val Asp
                     260                265                270
  20
        Asn Tyr Trp Ile Arg Ala Gln Pro Asn Lys Gly Arg Asn Gly Leu Ala
                     275                280                285
        Gly Thr Phe Ala Asn Gly Val Asn Ser Ala Ile Leu Arg Tyr Ala Gly
  25         290                295                300
        Ala Ala Asn Ala Asp Pro Thr Thr Ser Ala Asn Pro Asn Pro Ala Gln
        305                310                315                320
  30    Leu Asn Glu Ala Asp Leu His Ala Leu Ile Asp Pro Ala Ala Pro Gly
                     325                330                335
        Ile Pro Thr Pro Gly Ala Ala Asp Val Asn Leu Arg Phe Gln Leu Gly
                     340                345                350
  35
        Phe Ser Gly Gly Arg Phe Thr Ile Asn Gly Thr Ala Tyr Glu Ser Pro
                     355                360                365
        Ser Val Pro Thr Leu Leu Gln Ile Met Ser Gly Ala Gln Ser Ala Asn
  40         370                375                380
        Asp Leu Leu Pro Ala Gly Ser Val Tyr Glu Leu Pro Arg Asn Gln Val
        385                390                395                400
  45    Val Glu Leu Val Val Pro Ala Gly Val Leu Gly Gly Pro His Pro Phe
                     405                410                415
        His Leu His Gly His Ala Phe Ser Val Val Arg Ser Ala Gly Ser Ser
                     420                425                430
  50
        Thr Tyr Asn Phe Val Asn Pro Val Lys Arg Asp Val Val Ser Leu Gly
                     435                440                445
        Val Thr Gly Asp Glu Val Thr Ile Arg Phe Val Thr Asp Asn Pro Gly
  55         450                455                460
        Pro Trp Phe Phe His Cys His Ile Glu Phe His Leu Met Asn Gly Leu
        465                470                475                480
  60    Ala Ile Val Phe Ala Glu Asp Met Ala Asn Thr Val Asp Ala Asn Asn
                     485                490                495
        Pro Pro Val Glu Trp Ala Gln Leu Cys Glu Ile Tyr Asp Asp Leu Pro
                     500                505                510
  65
        Pro Glu Ala Thr Ser Ile Gln Thr Val Val Arg Arg Ala Glu Pro Thr
                     515                520                525
```

```
        Gly Phe Ser Ala Lys Phe Arg Arg Glu Gly Leu
            530                 535
```

5 (2) INFORMATION FOR SEQ ID NO: 2:

       (i) SEQUENCE CHARACTERISTICS:
           (A) LENGTH: 499 amino acids
           (B) TYPE: amino acid
10   (C) STRANDEDNESS: single
           (D) TOPOLOGY: linear

       (ii) MOLECULE TYPE: protein

15
       (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 2:

```
        Gly Ile Gly Pro Val Ala Asp Leu Thr Ile Thr Asn Ala Ala Val Ser
        1               5               10              15
20
        Pro Asp Gly Phe Ser Arg Gln Ala Val Val Val Asn Gly Gly Thr Pro
                    20              25              30

        Gly Pro Leu Ile Thr Gly Asn Met Gly Asp Arg Phe Gln Leu Asn Val
25              35              40              45

        Ile Asp Asn Leu Thr Asn His Thr Met Leu Lys Ser Thr Ser Ile His
            50              55              60

30      Trp His Gly Phe Phe Gln Lys Gly Thr Asn Trp Ala Asp Gly Pro Ala
        65              70              75              80

        Phe Ile Asn Gln Cys Pro Ile Ser Ser Gly His Ser Phe Leu Tyr Asp
                        85              90              95
35
        Phe Gln Val Pro Asp Gln Ala Gly Thr Phe Trp Tyr His Ser His Leu
                    100             105             110

        Ser Thr Gln Tyr Cys Asp Gly Leu Arg Gly Pro Phe Val Val Tyr Asp
40              115             120             125

        Pro Asn Asp Pro Ala Ala Asp Leu Tyr Asp Val Asp Asn Asp Asp Thr
            130             135             140

45      Val Ile Thr Leu Val Asp Trp Tyr His Val Ala Ala Lys Leu Gly Pro
        145             150             155             160

        Ala Phe Pro Leu Gly Ala Asp Ala Thr Leu Ile Asn Gly Lys Gly Arg
                    165             170             175
50
        Ser Pro Ser Thr Thr Thr Ala Asp Leu Ser Val Ile Ser Val Thr Pro
                    180             185             190

        Gly Lys Arg Tyr Arg Phe Arg Leu Val Ser Leu Ser Cys Asp Pro Asn
55                  195             200             205

        Tyr Thr Phe Ser Ile Asp Gly His Asn Met Thr Ile Ile Glu Thr Asp
            210             215             220

60      Ser Ile Asn Thr Ala Pro Leu Val Val Asp Ser Ile Gln Ile Phe Ala
        225             230             235             240

        Ala Gln Arg Tyr Ser Phe Val Leu Glu Ala Asn Gln Ala Val Asp Asn
                    245             250             255
65
        Tyr Trp Ile Arg Ala Asn Pro Asn Phe Gly Asn Val Gly Phe Thr Gly
                    260             265             270
```

```
        Gly Ile Asn Ser Ala Ile Leu Arg Tyr Asp Gly Ala Ala Ala Val Glu
            275                 280                 285

  5     Pro Thr Thr Thr Gln Thr Thr Ser Thr Ala Pro Leu Asn Glu Val Asn
            290                 295                 300

        Leu His Pro Leu Val Thr Thr Ala Val Pro Gly Ser Pro Val Ala Gly
        305                 310                 315                 320

 10     Gly Val Asp Leu Ala Ile Asn Met Ala Phe Asn Phe Asn Gly Thr Asn
                    325                 330                 335

        Phe Phe Ile Asn Gly Ala Ser Phe Thr Pro Pro Thr Val Pro Val Leu
                    340                 345                 350

 15     Leu Gln Ile Ile Ser Gly Ala Gln Asn Ala Gln Asp Leu Leu Pro Ser
                    355                 360                 365

        Gly Ser Val Tyr Ser Leu Pro Ser Asn Ala Asp Ile Glu Ile Ser Phe
 20         370                 375                 380

        Pro Ala Thr Ala Ala Ala Pro Gly Ala Pro His Pro Phe His Leu His
        385                 390                 395                 400

 25     Gly His Ala Phe Ala Val Val Arg Ser Ala Gly Ser Thr Val Tyr Asn
                    405                 410                 415

        Tyr Asp Asn Pro Ile Phe Arg Asp Val Val Ser Thr Gly Thr Pro Ala
                    420                 425                 430

 30     Ala Gly Asp Asn Val Thr Ile Arg Phe Arg Thr Asp Asn Pro Gly Pro
                435                 440                 445

        Trp Phe Leu His Cys His Ile Asp Phe His Leu Glu Ala Gly Phe Ala
 35         450                 455                 460

        Val Val Phe Ala Glu Asp Ile Pro Asp Val Ala Ser Ala Asn Pro Val
        465                 470                 475                 480

 40     Pro Gln Ala Trp Ser Asp Leu Cys Pro Thr Tyr Asp Ala Leu Asp Pro
                    485                 490                 495

        Ser Asp Gln

 45
    (2) INFORMATION FOR SEQ ID NO: 3:

        (i) SEQUENCE CHARACTERISTICS:
            (A) LENGTH: 499 amino acids
 50         (B) TYPE: amino acid
            (C) STRANDEDNESS: single
            (D) TOPOLOGY: linear

        (ii) MOLECULE TYPE: protein
 55

        (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 3:

        Ala Ile Gly Pro Val Ala Ser Leu Val Val Ala Asn Ala Pro Val Ser
 60     1               5                   10                  15

        Pro Asp Gly Phe Leu Arg Asp Ala Ile Val Val Asn Gly Val Val Pro
                    20                  25                  30

 65     Ser Pro Leu Ile Thr Gly Lys Lys Gly Asp Arg Phe Gln Leu Asn Val
                    35                  40                  45

        Val Asp Thr Leu Thr Asn His Ser Met Leu Lys Ser Thr Ser Ile His
```

```
               50                   55                   60

       Trp His Gly Phe Phe Gln Ala Gly Thr Asn Trp Ala Glu Gly Pro Ala
       65              70                   75              80
5
       Phe Val Asn Gln Cys Pro Ile Ala Ser Gly His Ser Phe Leu Tyr Asp
                       85                   90                   95

       Phe His Val Pro Asp Gln Ala Gly Thr Phe Trp Tyr His Ser His Leu
10                     100                 105                 110

       Ser Thr Gln Tyr Cys Asp Gly Leu Arg Gly Pro Phe Val Val Tyr Asp
               115                 120                 125

15     Pro Lys Asp Pro His Ala Ser Arg Tyr Asp Val Asp Asn Glu Ser Thr
               130                 135                 140

       Val Ile Thr Leu Thr Asp Trp Tyr His Thr Ala Ala Arg Leu Gly Pro
       145                 150                 155                 160
20
       Lys Phe Pro Leu Gly Ala Asp Ala Thr Leu Ile Asn Gly Leu Gly Arg
                       165                 170                 175

       Ser Ala Ser Thr Pro Thr Ala Ala Leu Ala Val Ile Asn Val Gln His
25                     180                 185                 190

       Gly Lys Arg Tyr Arg Phe Arg Leu Val Ser Ile Ser Cys Asp Pro Asn
               195                 200                 205

30     Tyr Thr Phe Ser Ile Asp Gly His Asn Leu Thr Val Ile Glu Val Asp
               210                 215                 220

       Gly Ile Asn Ser Gln Pro Leu Leu Val Asp Ser Ile Gln Ile Phe Ala
       225                 230                 235                 240
35
       Ala Gln Arg Tyr Ser Phe Val Leu Asn Ala Asn Gln Thr Val Gly Asn
                       245                 250                 255

       Tyr Trp Val Arg Ala Asn Pro Asn Phe Gly Thr Val Gly Phe Ala Gly
40                     260                 265                 270

       Gly Ile Asn Ser Ala Ile Leu Arg Tyr Gln Gly Ala Pro Val Ala Glu
               275                 280                 285

45     Pro Thr Thr Thr Gln Thr Pro Ser Val Ile Pro Leu Ile Glu Thr Asn
               290                 295                 300

       Leu His Pro Leu Ala Arg Met Pro Val Pro Gly Ser Pro Thr Pro Gly
       305                 310                 315                 320
50
       Gly Val Asp Lys Ala Leu Asn Leu Ala Phe Asn Phe Asn Gly Thr Asn
                       325                 330                 335

       Phe Phe Ile Asn Asn Ala Thr Phe Thr Pro Pro Thr Val Pro Val Leu
55                     340                 345                 350

       Leu Gln Ile Leu Ser Gly Ala Gln Thr Ala Gln Asp Leu Leu Pro Ala
               355                 360                 365

60     Gly Ser Val Tyr Pro Leu Pro Ala His Ser Thr Ile Glu Ile Thr Leu
               370                 375                 380

       Pro Ala Thr Ala Leu Ala Pro Gly Ala Pro His Pro Phe His Leu His
65     385                 390                 395                 400

       Gly His Ala Phe Ala Val Val Arg Ser Ala Gly Ser Thr Thr Tyr Asn
                       405                 410                 415
```

```
        Tyr Asn Asp Pro Ile Phe Arg Asp Val Val Ser Thr Gly Thr Pro Ala
                420             425             430

 5      Ala Gly Asp Asn Val Thr Ile Arg Phe Gln Thr Asp Asn Pro Gly Pro
                435             440             445

        Trp Phe Leu His Cys His Ile Asp Phe His Leu Asp Ala Gly Phe Ala
            450             455             460
10
        Ile Val Phe Ala Glu Asp Val Ala Asp Val Lys Ala Ala Asn Pro Val
        465             470             475             480

        Pro Lys Ala Trp Ser Asp Leu Cys Pro Ile Tyr Asp Gly Leu Ser Glu
15                      485             490             495

        Ala Asn Gln
```

20 (2) INFORMATION FOR SEQ ID NO: 4:

        (i) SEQUENCE CHARACTERISTICS:
              (A) LENGTH: 548 amino acids
              (B) TYPE: amino acid
25   (C) STRANDEDNESS: single
              (D) TOPOLOGY: linear

        (ii) MOLECULE TYPE: protein

30
        (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 4:

```
        Met His Thr Phe Leu Arg Ser Thr Ala Leu Val Val Ala Gly Leu Ser
        1               5               10              15
35
        Ala Arg Ala Leu Ala Ser Ile Gly Pro Val Thr Asp Phe His Ile Val
                20              25              30

        Asn Ala Ala Val Ser Pro Asp Gly Phe Ser Arg Gln Ala Val Leu Ala
40              35              40              45

        Glu Gly Val Phe Pro Gly Pro Leu Ile Ala Gly Asn Lys Gly Asp Asn
                50              55              60

45      Phe Gln Ile Asn Val Ile Asp Glu Leu Thr Asn Ala Thr Met Leu Lys
        65              70              75              80

        Thr Thr Thr Ile His Trp His Gly Phe Phe Gln His Gly Thr Asn Trp
                        85              90              95
50
        Ala Asp Gly Pro Ala Phe Ile Asn Gln Cys Pro Ile Ala Ser Gly Asp
                100             105             110

        Ser Phe Leu Tyr Asn Phe Gln Val Pro Asp Gln Ala Gly Thr Phe Trp
55          115             120             125

        Tyr His Ser His Leu Ser Thr Gln Tyr Cys Asp Gly Leu Arg Gly Pro
            130             135             140

60      Phe Val Val Tyr Asp Pro Ala Asp Pro Tyr Leu Asp Gln Tyr Asp Val
        145             150             155             160

        Asp Asp Asp Ser Thr Val Ile Thr Leu Ala Asp Trp Tyr His Thr Ala
                        165             170             175
65
        Ala Arg Leu Gly Ser Pro Phe Pro Ala Ala Asp Thr Thr Leu Ile Asn .
                180             185             190
```

```
        Gly Leu Gly Arg Cys Gly Glu Ala Gly Cys Pro Val Ser Asp Leu Ala
                195                 200             205

 5      Val Ile Ser Val Thr Lys Gly Lys Arg Tyr Arg Phe Arg Leu Val Ser
                210             215             220

        Ile Ser Cys Asp Ser Phe Phe Thr Phe Ser Ile Asp Gly His Ser Leu
        225             230                 235                 240

10      Asn Val Ile Glu Val Asp Ala Thr Asn His Gln Pro Leu Thr Val Asp
                        245             250                 255

        Glu Leu Thr Ile Tyr Ala Gly Gln Arg Tyr Ser Phe Ile Leu Thr Ala
                    260             265                 270

15      Asp Gln Asp Val Asp Asn Tyr Trp Ile Arg Ala Asn Pro Gly Ile Gly
                    275             280             285

        Ile Thr Thr Gly Phe Ala Gly Gly Ile Asn Ser Ala Ile Leu Arg Tyr
20          290             295                 300

        Asp Gly Ala Asp Val Val Glu Pro Thr Thr Thr Gln Ala Thr Ser Pro
        305             310                 315                 320

25      Val Val Leu Ser Glu Ser Asn Leu Ala Pro Leu Thr Asn Ala Ala Ala
                    325                 330                 335

        Pro Gly Leu Pro Glu Val Gly Gly Val Asp Leu Ala Leu Asn Phe Asn
                    340             345                 350

30      Leu Thr Phe Asp Gly Pro Ser Leu Lys Phe Gln Ile Asn Gly Val Thr
                    355             360                 365

        Phe Val Pro Pro Thr Val Pro Val Leu Leu Gln Ile Leu Ser Gly Ala
35          370             375                 380

        Gln Ser Ala Ala Asp Leu Leu Pro Ser Gly Ser Val Tyr Ala Leu Pro
        385                 390                 395                 400

40      Ser Asn Ala Thr Ile Glu Leu Ser Leu Pro Ala Gly Ala Leu Gly Gly
                    405                 410                 415

        Pro His Pro Phe His Leu His Gly His Thr Phe Ser Val Val Arg Pro
                    420             425                 430

45      Ala Gly Ser Thr Thr Tyr Asn Tyr Val Asn Pro Val Gln Arg Asp Val
                    435             440                 445

        Val Ser Ile Gly Asn Thr Gly Asp Asn Val Thr Ile Arg Phe Asp Thr
50          450             455                 460

        Asn Asn Pro Gly Pro Trp Phe Leu His Cys His Ile Asp Trp His Leu
        465             470                 475                 480

55      Glu Ala Ala Leu Pro Leu Ser Ser Leu Arg Thr Ser Leu Thr Leu Arg
                    485             490                 495

        Pro Leu Thr Leu Ser Pro Arg Thr Gly Pro Thr Cys Ala Leu Ser Thr
                    500             505             510

60      Thr Leu Trp Thr His Leu Ile Thr Ser Gly Phe Ala Ser Ile Ile Gln
                    515             520                 525

65      Trp Met Met Gly Gly Asn Gly Leu Phe Ala Pro His Ala Leu Ser Phe
                530             535                 540

        Leu Gly Ser Gln
```

545

(2) INFORMATION FOR SEQ ID NO: 5:

        (i) SEQUENCE CHARACTERISTICS:
             (A) LENGTH: 529 amino acids
             (B) TYPE: amino acid
             (C) STRANDEDNESS: single
             (D) TOPOLOGY: linear

      (ii) MOLECULE TYPE: protein

      (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 5:

Met Leu Ser Ser Ile Thr Leu Leu Pro Leu Leu Ala Ala Val Ser Thr
1   5   10   15

Pro Ala Phe Ala Ala Val Arg Asn Tyr Lys Phe Asp Ile Lys Asn Val
            20   25   30

Asn Val Ala Pro Asp Gly Phe Gln Arg Ser Ile Val Ser Val Asn Gly
        35   40   45

Leu Val Pro Gly Thr Leu Ile Thr Ala Asn Lys Gly Asp Thr Leu Arg
    50   55   60

Ile Asn Val Thr Asn Gln Leu Thr Asp Pro Ser Met Arg Arg Ala Thr
65   70   75   80

Thr Ile His Trp His Gly Leu Phe Gln Ala Thr Thr Ala Asp Glu Asp
                85   90   95

Gly Pro Ala Phe Val Thr Gln Cys Pro Ile Ala Gln Asn Leu Ser Tyr
            100   105   110

Thr Tyr Glu Ile Pro Leu Arg Gly Gln Thr Gly Thr Met Trp Tyr His
        115   120   125

Ala His Leu Ala Ser Gln Tyr Val Asp Gly Leu Arg Gly Pro Leu Val
    130   135   140

Ile Tyr Asp Pro Asn Asp Pro His Lys Ser Arg Tyr Asp Val Asp Asp
145   150   155   160

Ala Ser Thr Val Val Met Leu Glu Asp Trp Tyr His Thr Pro Ala Pro
                165   170   175

Val Leu Glu Lys Gln Met Phe Ser Thr Asn Asn Thr Ala Leu Leu Ser
            180   185   190

Pro Val Pro Asp Ser Gly Leu Ile Asn Gly Lys Gly Arg Tyr Val Gly
        195   200   205

Gly Pro Ala Val Pro Arg Ser Val Ile Asn Val Lys Arg Gly Lys Arg
    210   215   220

Tyr Arg Leu Arg Val Ile Asn Ala Ser Ala Ile Gly Ser Phe Thr Phe
225   230   235   240

Ser Ile Glu Gly His Ser Leu Thr Val Ile Glu Ala Asp Gly Ile Leu
                245   250   255

His Gln Pro Leu Ala Val Asp Ser Phe Gln Ile Tyr Ala Gly Gln Arg
            260   265   270

Tyr Ser Val Ile Val Glu Ala Asn Gln Thr Ala Ala Asn Tyr Trp Ile
        275   280   285

```
     Arg Ala Pro Met Thr Val Ala Gly Ala Gly Thr Asn Ala Asn Leu Asp
         290             295             300

 5   Pro Thr Asn Val Phe Ala Val Leu His Tyr Glu Gly Ala Pro Asn Ala
     305             310             315                         320

     Glu Pro Thr Thr Glu Gln Gly Ser Ala Ile Gly Thr Ala Leu Val Glu
                     325             330             335
10
     Glu Asn Leu His Ala Leu Ile Asn Pro Gly Ala Pro Gly Gly Ser Ala
                     340             345             350

     Pro Ala Asp Val Ser Leu Asn Leu Ala Ile Gly Arg Ser Thr Val Asp
15                   355             360             365

     Gly Ile Leu Arg Phe Thr Phe Asn Asn Ile Lys Tyr Glu Ala Pro Ser
         370             375             380

20   Leu Pro Thr Leu Leu Lys Ile Leu Ala Asn Asn Ala Ser Asn Asp Ala
     385             390             395             400

     Asp Phe Thr Pro Asn Glu His Thr Ile Val Leu Pro His Asn Lys Val
                     405             410             415
25
     Ile Glu Leu Asn Ile Thr Gly Gly Ala Asp His Pro Ile His Leu His
                     420             425             430

     Gly His Val Phe Asp Ile Val Lys Ser Leu Gly Gly Thr Pro Asn Tyr
30                   435             440             445

     Val Asn Pro Pro Arg Arg Asp Val Val Arg Val Gly Gly Thr Gly Val
         450             455             460

35   Val Leu Arg Phe Lys Thr Asp Asn Pro Gly Pro Trp Phe Val His Cys
     465             470             475             480

     His Ile Asp Trp His Leu Glu Ala Gly Leu Ala Leu Val Phe Ala Glu
                     485             490             495
40
     Ala Pro Ser Gln Ile Arg Gln Gly Val Gln Ser Val Gln Pro Asn Asn
                     500             505             510

     Ala Trp Asn Gln Leu Cys Pro Lys Tyr Ala Ala Leu Pro Pro Asp Leu
45                   515             520             525

     Gln
```

50 (2) INFORMATION FOR SEQ ID NO: 6:

        (i) SEQUENCE CHARACTERISTICS:
             (A) LENGTH: 599 amino acids
             (B) TYPE: amino acid
55   (C) STRANDEDNESS: single
             (D) TOPOLOGY: linear

        (ii) MOLECULE TYPE: protein

60   (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 6:

```
     Met Ala Arg Ser Thr Thr Ser Leu Phe Ala Leu Ser Leu Val Ala Ser
     1               5               10              15

65   Ala Phe Ala Arg Val Val Asp Tyr Gly Phe Asp Val Ala Asn Gly Ala
                     20              25              30

     Val Ala Pro Asp Gly Val Thr Arg Asn Ala Val Leu Val Asn Gly Arg
```

```
              35                    40                    45
      Phe Pro Gly Pro Leu Ile Thr Ala Asn Lys Gly Asp Thr Leu Lys Ile
          50                      55                  60
 5
      Thr Val Arg Asn Lys Leu Ser Asp Pro Thr Met Arg Arg Ser Thr Thr
      65                      70                  75                  80

      Ile His Trp His Gly Leu Leu Gln His Arg Thr Ala Glu Glu Asp Gly
10                        85                  90                  95

      Pro Ala Phe Val Thr Gln Cys Pro Ile Pro Pro Gln Glu Ser Tyr Thr
                  100                     105                 110
15
      Tyr Thr Met Pro Leu Gly Glu Gln Thr Gly Thr Tyr Trp Tyr His Ser
              115                     120                 125

      His Leu Ser Ser Gln Tyr Val Asp Gly Leu Arg Gly Pro Ile Val Ile
20        130                     135                 140

      Tyr Asp Pro His Asp Pro Tyr Arg Asn Tyr Tyr Asp Val Asp Asp Glu
      145                     150                 155                 160

      Arg Thr Val Phe Thr Leu Ala Asp Trp Tyr His Thr Pro Ser Glu Ala
25                165                     170                 175

      Ile Ile Ala Thr His Asp Val Leu Lys Thr Ile Pro Asp Ser Gly Thr
                  180                     185                 190

      Ile Asn Gly Lys Gly Lys Tyr Asp Pro Ala Ser Ala Asn Thr Asn Asn
30            195                     200                 205

      Thr Thr Leu Glu Asn Leu Tyr Thr Leu Lys Val Lys Arg Gly Lys Arg
          210                     215                 220
35
      Tyr Arg Leu Arg Ile Ile Asn Ala Ser Ala Ile Ala Ser Phe Arg Phe
      225         .           230                 235                 240

      Gly Val Gln Gly His Lys Cys Thr Ile Ile Glu Ala Asp Gly Val Leu
40                245                     250                 255

      Thr Lys Pro Ile Glu Val Asp Ala Phe Asp Ile Leu Ala Gly Gln Arg
                  260                     265                 270

      Tyr Ser Cys Ile Leu Lys Ala Asp Gln Asp Pro Asp Ser Tyr Trp Ile
45            275                     280                 285

      Asn Ala Pro Ile Thr Asn Val Leu Asn Thr Asn Val Gln Ala Leu Leu
          290                     295                 300
50
      Val Tyr Glu Asp Asp Lys Arg Pro Thr His Tyr Pro Trp Lys Pro Phe
      305                     310                 315                 320

      Leu Thr Trp Lys Ile Ser Asn Glu Ile Ile Gln Tyr Trp Gln His Lys
55                325                     330                 335

      His Gly Ser His Gly His Lys Gly Lys Gly His His His Lys Val Arg
                  340                     345                 350
      Ala Ile Gly Gly Val Ser Gly Leu Ser Ser Arg Val Lys Ser Arg Ala
60            355                     360                 365

      Ser Asp Leu Ser Lys Lys Ala Val Glu Leu Ala Ala Ala Leu Val Ala
          370                     375                 380

65    Gly Glu Ala Glu Leu Asp Lys Arg Gln Asn Glu Asp Asn Ser Thr Ile
      385                     390                 395                 400

      Val Leu Asp Glu Thr Lys Leu Ile Pro Leu Val Gln Pro Gly Ala Pro
```

```
                   405                    410                    415

     Gly Gly Ser Arg Pro Ala Asp Val Val Val Pro Leu Asp Phe Gly Leu
                 420         425             430
 5
     Asn Phe Ala Asn Gly Leu Trp Thr Ile Asn Asn Val Ser Tyr Ser Pro
                 435             440             445
     Pro Asp Val Pro Thr Leu Leu Lys Ile Leu Thr Asp Lys Asp Lys Val
10       450             455             460
     Asp Ala Ser Asp Phe Thr Ala Asp Glu His Thr Tyr Ile Leu Pro Lys
     465             470             475                         480
15   Asn Gln Val Val Glu Leu His Ile Lys Gly Gln Ala Leu Gly Ile Val
                 485             490             495
     His Pro Leu His Leu His Gly His Ala Phe Asp Val Val Gln Phe Gly
                 500             505             510
20
     Asp Asn Ala Pro Asn Tyr Val Asn Pro Pro Arg Arg Asp Val Val Gly
                 515             520             525
     Val Thr Asp Ala Gly Val Arg Ile Gln Phe Arg Thr Asp Asn Pro Gly
25       530             535             540
     Pro Trp Phe Leu His Cys His Ile Asp Trp His Leu Glu Glu Gly Phe
     545             550             555                         560
30   Ala Met Val Phe Ala Glu Ala Pro Glu Asp Ile Lys Lys Gly Ser Gln
                 565             570             575
     Ser Val Lys Pro Asp Gly Gln Trp Lys Lys Leu Cys Glu Lys Tyr Glu
                 580             585             590
35
     Lys Leu Pro Glu Ala Leu Gln
                 595
```

(2) INFORMATION FOR SEQ ID NO: 7:

     (i) SEQUENCE CHARACTERISTICS:
         (A) LENGTH: 572 amino acids
         (B) TYPE: amino acid
         (C) STRANDEDNESS: single
         (D) TOPOLOGY: linear

     (ii) MOLECULE TYPE: protein

     (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 7:

```
     Met Ala Arg Thr Thr Phe Leu Val Ser Val Ser Leu Phe Val Ser Ala
     1           5               10              15
     Val Leu Ala Arg Thr Val Glu Tyr Asn Leu Lys Ile Ser Asn Gly Lys
                 20              25              30
     Ile Ala Pro Asp Gly Val Glu Arg Asp Ala Thr Leu Val Asn Gly Gly
                 35              40              45
     Tyr Pro Gly Pro Leu Ile Phe Ala Asn Lys Gly Asp Thr Leu Lys Val
                 50              55              60
     Lys Val Gln Asn Lys Leu Thr Asn Pro Asp Met Tyr Arg Thr Thr Ser
     65              70              75              80
     Ile His Trp His Gly Leu Leu Gln His Arg Asn Ala Asp Asp Asp Gly
                 85              90              95
```

```
        Pro Ala Phe Val Thr Gln Cys Pro Ile Val Pro Gln Ala Ser Tyr Thr
                    100             105             110

  5     Tyr Thr Met Pro Leu Gly Asp Gln Thr Gly Thr Tyr Trp Tyr His Ser
                    115             120             125

        His Leu Ser Ser Gln Tyr Val Asp Gly Leu Arg Gly Pro Leu Val Ile
                    130             135             140
 10
        Tyr Asp Pro Lys Asp Pro His Arg Arg Leu Tyr Asp Ile Asp Asp Glu
        145             150             155             160

 15     Lys Thr Val Leu Ile Ile Gly Asp Trp Tyr His Thr Ser Ser Lys Ala
                    165             170             175

        Ile Leu Ala Thr Gly Asn Ile Thr Leu Gln Gln Pro Asp Ser Ala Thr
                    180             185             190
 20
        Ile Asn Gly Lys Gly Arg Phe Asp Pro Asp Asn Thr Pro Ala Asn Pro
                    195             200             205

        Asn Thr Leu Tyr Thr Leu Lys Val Lys Arg Gly Lys Arg Tyr Arg Leu
                    210             215             220
 25
        Arg Val Ile Asn Ser Ser Ala Ile Ala Ser Phe Arg Met Ser Ile Gln
        225             230             235             240

        Gly His Lys Met Thr Val Ile Ala Ala Asp Gly Val Ser Thr Lys Pro
 30                 245             250             255

        Tyr Gln Val Asp Ser Phe Asp Ile Leu Ala Gly Gln Arg Ile Asp Ala
                    260             265             270

 35     Val Val Glu Ala Asn Gln Glu Pro Asp Thr Tyr Trp Ile Asn Ala Pro
                    275             280             285

        Leu Thr Asn Val Ala Asn Lys Thr Ala Gln Ala Leu Leu Ile Tyr Glu
                    290             295             300
 40
        Asp Asp Arg Arg Pro Tyr His Pro Pro Lys Gly Pro Tyr Arg Lys Trp
        305             310             315             320

        Ser Val Ser Glu Ala Ile Ile Lys Tyr Trp Lys His Lys His Gly Arg
 45                 325             330                 335

        Gly Leu Leu Ser Gly His Gly Gly Leu Lys Ala Arg Met Met Glu Gly
                    340             345             350

 50     Ser Leu His Leu His Gly Arg Arg Asp Ile Val Lys Arg Gln Asn Glu
                    355             360             365

        Thr Thr Thr Val Val Met Asp Glu Thr Lys Leu Val Pro Leu Glu His
                    370             375             380
 55
        Pro Gly Ala Ala Cys Gly Ser Lys Pro Ala Asp Leu Val Ile Asp Leu
        385             390             395             400

 60     Thr Phe Gly Val Asn Phe Thr Thr Gly His Trp Met Ile Asn Gly Ile
                    405             410             415

        Pro His Lys Ser Pro Asp Met Pro Thr Leu Leu Lys Ile Leu Thr Asp
                    420             425             430
 65
        Thr Asp Gly Val Thr Glu Ser Asp Phe Thr Gln Pro Glu His Thr Ile
                    435             440             445
```

```
        Ile Leu Pro Lys Asn Lys Cys Val Glu Phe Asn Ile Lys Gly Asn Ser
            450             455             460

    5   Gly Leu Gly Ile Val His Pro Ile His Leu His Gly His Thr Phe Asp
        465             470             475             480

        Val Val Gln Phe Gly Asn Asn Pro Pro Asn Tyr Val Asn Pro Pro Arg
                    485             490             495

   10   Arg Asp Val Val Gly Ala Thr Asp Glu Gly Val Arg Phe Gln Phe Lys
                    500             505             510

        Thr Asp Asn Pro Gly Pro Trp Phe Leu His Cys His Ile Asp Trp His
                515             520             525

   15   Leu Glu Glu Gly Phe Ala Met Val Phe Ala Glu Ala Pro Glu Ala Ile
            530             535             540

   20   Lys Gly Gly Pro Lys Ser Val Pro Val Asp Arg Gln Trp Lys Asp Leu
        545             550             555             560

        Cys Arg Lys Tyr Gly Ser Leu Pro Ala Gly Phe Leu
                    565             570
```

25 (2) INFORMATION FOR SEQ ID NO: 8:

        (i) SEQUENCE CHARACTERISTICS:
            (A) LENGTH: 575 amino acids
            (B) TYPE: amino acid
   30   (C) STRANDEDNESS: single
            (D) TOPOLOGY: linear

        (ii) MOLECULE TYPE: protein

   35

        (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 8:

```
        Met Ala Arg Thr Thr Phe Leu Val Ser Val Ser Leu Phe Val Ser Ala
        1               5               10              15
   40
        Val Leu Ala Arg Thr Val Glu Tyr Gly Leu Lys Ile Ser Asp Gly Glu
                    20              25              30

        Ile Ala Pro Asp Gly Val Lys Arg Asn Ala Thr Leu Val Asn Gly Gly
   45       35              40              45

        Tyr Pro Gly Pro Leu Ile Phe Ala Asn Lys Gly Asp Thr Leu Lys Val
            50              55              60

   50   Lys Val Gln Asn Lys Leu Thr Asn Pro Glu Met Tyr Arg Thr Thr Ser
        65              70              75              80

        Ile His Trp His Gly Leu Leu Gln His Arg Asn Ala Asp Asp Asp Gly
                        85              90              95
   55
        Pro Ser Phe Val Thr Gln Cys Pro Ile Val Pro Arg Glu Ser Tyr Thr
                    100             105             110

        Tyr Thr Ile Pro Leu Asp Asp Gln Thr Gly Thr Tyr Trp Tyr His Ser
   60           115             120             125

        His Leu Ser Ser Gln Tyr Val Asp Gly Leu Arg Gly Pro Leu Val Ile
            130             135             140

   65   Tyr Pro Lys Asp Pro His Arg Arg Leu Tyr Asp Val Asp Asp Glu Lys
        145             150             155             160

        Thr Val Leu Ile Ile Gly Asp Trp Tyr His Glu Ser Ser Lys Ala Ile
```

```
                    165                 170                 175
         Leu Ala Ser Gly Asn Ile Thr Arg Gln Arg Pro Val Ser Ala Thr Ile
                     180                 185                 190
  5
         Asn Gly Lys Gly Arg Phe Asp Pro Asp Asn Thr Pro Ala Asn Pro Asp
                     195                 200                 205
 10      Thr Leu Tyr Thr Leu Lys Val Lys Arg Gly Lys Arg Tyr Arg Leu Arg
             210                 215                 220
         Val Ile Asn Ser Ser Glu Ile Ala Ser Phe Arg Phe Ser Val Glu Gly
         225                 230                 235                 240
 15      His Lys Val Thr Val Ile Ala Ala Asp Gly Val Ser Thr Lys Pro Tyr
                     245                 250                 255
         Gln Val Asp Ala Phe Asp Ile Leu Ala Gly Gln Arg Ile Asp Cys Val
                     260                 265                 270
 20      Val Glu Ala Asn Gln Glu Pro Asp Thr Tyr Trp Ile Asn Ala Pro Leu
                     275                 280                 285
         Thr Asn Val Pro Asn Lys Thr Ala Gln Ala Leu Leu Val Tyr Glu Glu
             290                 295                 300
 25      Asp Arg Arg Pro Tyr His Pro Pro Lys Gly Pro Tyr Arg Lys Trp Ser
         305                 310                 315                 320
 30      Val Ser Glu Ala Ile Ile Lys Tyr Trp Asn His Lys His Lys His Gly
                     325                 330                 335
         Arg Gly Leu Leu Ser Gly His Gly Gly Leu Lys Ala Arg Met Ile Glu
                     340                 345                 350
 35      Gly Ser His His Leu His Ser Arg Ser Val Val Lys Arg Gln Asn Glu
                 355                 360                 365
         Thr Thr Thr Val Val Met Asp Glu Ser Lys Leu Val Pro Leu Glu Tyr
 40          370                 375                 380
         Pro Gly Ala Ala Cys Gly Ser Lys Pro Ala Asp Leu Val Leu Asp Leu
         385                 390                 395                 400
 45      Thr Phe Gly Leu Asn Phe Ala Thr Gly His Trp Met Ile Asn Gly Ile
                     405                 410                 415
         Pro Tyr Glu Ser Pro Lys Ile Pro Thr Leu Leu Lys Ile Leu Thr Asp
                     420                 425                 430
 50      Glu Asp Gly Val Thr Glu Ser Asp Phe Thr Lys Glu Glu His Thr Val
                 435                 440                 445
 55      Ile Leu Pro Lys Asn Lys Cys Ile Glu Phe Asn Ile Lys Gly Asn Ser
             450                 455                 460
         Gly Ile Pro Ile Thr His Pro Val His Leu His Gly His Thr Trp Asp
         465                 470                 475                 480
 60      Val Val Gln Phe Gly Asn Asn Pro Pro Asn Tyr Val Asn Pro Pro Arg
                     485                 490                 495
         Arg Asp Val Val Gly Ser Thr Asp Ala Gly Val Arg Ile Gln Phe Lys
 65          500                 505                 510
         Thr Asp Asn Pro Gly Pro Trp Phe Leu His Cys His Ile Asp Trp His
             515                 520                 525
```

```
        Leu Glu Glu Gly Phe Ala Met Val Phe Ala Glu Ala Pro Glu Ala Val
            530             535             540

5       Lys Gly Gly Pro Lys Ser Val Ala Val Asp Ser Gln Trp Glu Gly Leu
            545             550             555             560

        Cys Gly Lys Tyr Asp Asn Trp Leu Lys Ser Asn Pro Gly Gln Leu
                        565             570             575
10
    (2) INFORMATION FOR SEQ ID NO: 9:

        (i) SEQUENCE CHARACTERISTICS:
            (A) LENGTH: 616 amino acids
15          (B) TYPE: amino acid
            (C) STRANDEDNESS: single
            (D) TOPOLOGY: linear

        (ii) MOLECULE TYPE: protein
20

        (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 9:

        Met Lys Arg Phe Phe Ile Asn Ser Leu Leu Leu Leu Ala Gly Leu Leu
25      1               5               10              15

        Asn Ser Gly Ala Leu Ala Ala Pro Ser Thr His Pro Arg Ser Asn Pro
                        20              25              30

30      Asp Ile Leu Leu Glu Arg Asp Asp His Ser Leu Thr Ser Arg Gln Gly
                    35              40              45

        Ser Cys His Ser Pro Ser Asn Arg Ala Cys Trp Cys Ser Gly Phe Asp
                50              55              60
35
        Ile Asn Thr Asp Tyr Glu Thr Lys Thr Pro Asn Thr Gly Val Val Arg
        65              70              75              80

        Arg Tyr Thr Phe Asp Ile Thr Glu Val Asp Asn Arg Pro Gly Pro Asp
40                      85              90              95

        Gly Val Ile Lys Glu Lys Leu Met Leu Ile Asn Asp Lys Leu Leu Gly
                        100             105             110

45      Pro Thr Val Phe Ala Asn Trp Gly Asp Thr Ile Glu Val Thr Val Asn
                    115             120             125

        Asn His Leu Arg Thr Asn Gly Thr Ser Ile His Trp His Gly Leu His
            130             135             140
50
        Gln Lys Gly Thr Asn Tyr His Asp Gly Ala Asn Gly Val Thr Glu Cys
        145             150             155             160

        Pro Ile Pro Pro Gly Gly Ser Arg Val Tyr Ser Phe Arg Ala Arg Gln
55                      165             170             175

        Tyr Gly Thr Ser Trp Tyr His Ser His Phe Ser Ala Gln Tyr Gly Asn
                        180             185             190

60      Gly Val Ser Gly Ala Ile Gln Ile Asn Gly Pro Ala Ser Leu Pro Tyr
                    195             200             205

        Asp Ile Asp Leu Gly Val Leu Pro Leu Xaa Asp Trp Tyr Tyr Lys Ser
            210             215             220
65
        Ala Asp Gln Leu Val Ile Glu Thr Leu Xaa Lys Gly Asn Ala Pro Phe
        225             230             235             240
```

```
        Ser Asp Asn Val Leu Ile Asn Gly Thr Ala Lys His Pro Thr Thr Gly
                    245                 250                 255

  5     Glu Gly Glu Tyr Ala Ile Val Lys Leu Thr Pro Asp Lys Arg His Arg
                    260                 265                 270

        Leu Arg Leu Ile Asn Met Ser Val Glu Asn His Phe Gln Val Ser Leu
                    275                 280                 285

 10     Ala Lys His Thr Met Thr Val Ile Ala Ala Asp Met Val Pro Val Asn
                    290                 295                 300

        Ala Met Thr Val Asp Ser Leu Phe Met Ala Val Gly Gln Arg Tyr Asp
        305                 310                 315                 320

 15     Val Thr Ile Asp Ala Ser Gln Ala Val Gly Asn Tyr Trp Phe Asn Ile
                    325                 330                 335

        Thr Phe Gly Gly Gln Gln Lys Cys Gly Phe Ser His Asn Pro Ala Pro
 20                 340                 345                 350

        Ala Ala Ile Phe Arg Tyr Glu Gly Ala Pro Asp Ala Leu Pro Thr Asp
                    355                 360                 365

 25     Pro Gly Ala Ala Pro Lys Asp His Gln Cys Leu Asp Thr Leu Asp Leu
                    370                 375                 380

        Ser Pro Val Val Gln Lys Asn Val Pro Val Asp Gly Phe Val Lys Glu
        385                 390                 395                 400
 30
        Pro Gly Asn Thr Leu Pro Val Thr Leu His Val Asp Gln Ala Ala Ala
                    405                 410                 415

 35     Pro His Val Phe Thr Trp Lys Ile Asn Gly Ser Ala Ala Asp Val Asp
                    420                 425                 430

        Trp Asp Arg Pro Val Leu Glu Tyr Val Met Asn Asn Asp Leu Ser Ser
                    435                 440                 445

 40     Ile Pro Val Lys Asn Asn Ile Val Arg Val Asp Gly Val Asn Glu Trp
                    450                 455                 460

        Thr Tyr Trp Leu Val Glu Asn Asp Pro Glu Gly Arg Leu Ser Leu Pro
        465                 470                 475                 480
 45
        His Pro Met His Leu His Gly His Asp Phe Phe Val Leu Gly Arg Ser
                    485                 490                 495

        Pro Asp Val Ser Pro Asp Ser Glu Thr Arg Phe Val Phe Asp Pro Ala
 50                 500                 505                 510


        Val Asp Leu Pro Arg Leu Arg Gly His Asn Pro Val Arg Arg Asp Val
                    515                 520                 525
 55
        Thr Met Leu Pro Ala Arg Gly Trp Leu Leu Leu Ala Phe Arg Thr Asp
                    530                 535                 540

        Asn Pro Gly Ala Trp Leu Phe His Cys His Ile Ala Xaa His Val Ser
 60     545                 550                 555                 560

        Gly Gly Leu Ser Val Asp Phe Leu Glu Arg Pro Asp Glu Leu Arg Gly
                    565                 570                 575

 65     Gln Leu Thr Gly Glu Ser Lys Ala Glu Leu Glu Arg Val Cys Arg Glu
                    580                 585                 590

        Trp Lys Asp Trp Glu Ala Lys Ser Pro His Gly Lys Ile Asp Ser Gly
```

```
                595                   600                   605

        Leu Lys Gln Arg Arg Trp Asp Ala
            610                 615
```

(2) INFORMATION FOR SEQ ID NO: 10:

    (i) SEQUENCE CHARACTERISTICS:
        (A) LENGTH: 573 amino acids
        (B) TYPE: amino acid
        (C) STRANDEDNESS: single
        (D) TOPOLOGY: linear

    (ii) MOLECULE TYPE: protein

    (xi) SEQUENCE DESCRIPTION: SEQ ID NO: 10:

```
    Gln Gln Ser Cys Asn Thr Pro Ser Asn Arg Ala Cys Trp Thr Asp Gly
    1               5                   10                  15

    Tyr Asp Ile Asn Thr Asp Tyr Glu Val Asp Ser Pro Asp Thr Gly Val
                20                  25                  30

    Val Arg Pro Tyr Thr Leu Thr Leu Thr Glu Val Asp Asn Trp Thr Gly
            35                  40                  45

    Pro Asp Gly Val Val Lys Glu Lys Val Met Leu Val Asn Asn Ser Ile
            50                  55                  60

    Ile Gly Pro Thr Ile Phe Ala Asp Trp Gly Asp Thr Ile Gln Val Thr
    65                  70                  75                  80

    Val Ile Asn Asn Leu Glu Thr Asn Gly Thr Ser Ile His Trp His Gly
                    85                  90                  95

    Leu His Gln Lys Gly Thr Asn Leu His Asp Gly Ala Asn Gly Ile Thr
                100                 105                 110

    Glu Cys Pro Ile Pro Pro Lys Gly Gly Arg Lys Val Tyr Arg Phe Lys
                115                 120                 125

    Ala Gln Gln Tyr Gly Thr Ser Trp Tyr His Ser His Phe Ser Ala Gln
                130                 135                 140

    Tyr Gly Asn Gly Val Val Gly Ala Ile Gln Ile Asn Gly Pro Ala Ser
    145                 150                 155                 160

    Leu Pro Tyr Asp Thr Asp Leu Gly Val Phe Pro Ile Ser Asp Tyr Tyr
                    165                 170                 175

    Tyr Ser Ser Ala Asp Glu Leu Val Glu Leu Thr Lys Asn Ser Gly Ala
                180                 185                 190

    Pro Phe Ser Asp Asn Val Leu Phe Asn Gly Thr Ala Lys His Pro Glu
                195                 200                 205

    Thr Gly Glu Gly Glu Tyr Ala Asn Val Thr Leu Thr Pro Gly Arg Arg
                210                 215                 220

    His Arg Leu Arg Leu Ile Asn Thr Ser Val Glu Asn His Phe Gln Val
    225                 230                 235                 240

    Ser Leu Val Asn His Thr Met Cys Ile Ile Ala Ala Asp Met Val Pro
                    245                 250                 255

    Val Asn Ala Met Thr Val Asp Ser Leu Phe Leu Gly Val Gly Gln Arg
                260                 265                 270
```

```
       Tyr Asp Val Val Ile Glu Ala Asn Arg Thr Pro Gly Asn Tyr Trp Phe
           275                 280                 285

 5     Asn Val Thr Phe Gly Gly Gly Leu Leu Cys Gly Gly Ser Arg Asn Pro
           290             295             300

       Tyr Pro Ala Ala Ile Phe His Tyr Ala Gly Ala Pro Gly Gly Pro Pro
       305             310             315             320

10     Thr Asp Glu Gly Lys Ala Pro Val Asp His Asn Cys Leu Asp Leu Pro
                   325             330             335

       Asn Leu Lys Pro Val Val Ala Arg Asp Val Pro Leu Ser Gly Phe Ala
15             340             345             350

       Lys Arg Ala Asp Asn Thr Leu Asp Val Thr Leu Asp Thr Thr Gly Thr
               355             360             365

20     Pro Leu Phe Val Trp Lys Val Asn Gly Ser Ala Ile Asn Ile Asp Trp
           370             375             380

       Gly Arg Ala Val Val Asp Tyr Val Leu Thr Gln Asn Thr Ser Phe Pro
       385             390             395             400

25     Pro Gly Tyr Asn Ile Val Glu Val Asn Gly Ala Asp Gln Trp Ser Tyr
                   405             410             415

       Trp Leu Ile Glu Asn Asp Pro Gly Ala Pro Phe Thr Leu Pro His Pro
30             420             425             430

       Met His Leu His Gly His Asp Phe Tyr Val Leu Gly Arg Ser Pro Asp
               435             440             445

35     Glu Ser Pro Ala Ser Asn Glu Arg His Val Phe Asp Pro Ala Arg Asp
           450             455             460

       Ala Gly Leu Leu Ser Gly Ala Asn Pro Val Arg Arg Asp Val Ser Met
       465             470             475             480

40     Leu Pro Ala Phe Gly Trp Val Val Leu Ser Phe Arg Ala Asp Asn Pro
                   485             490             495

       Gly Ala Trp Leu Phe His Cys His Ile Ala Trp His Val Ser Gly Gly
45             500             505             510

       Leu Gly Val Val Tyr Leu Glu Arg Ala Asp Asp Leu Arg Gly Ala Val
               515             520             525

50
       Ser Asp Ala Asp Ala Asp Asp Leu Asp Arg Leu Cys Ala Asp Trp Arg
           530             535             540

55     Arg Tyr Trp Pro Thr Asn Pro Tyr Pro Lys Ser Asp Ser Gly Leu Lys
       545             550             555             560

       His Arg Trp Val Glu Glu Gly Glu Trp Leu Val Lys Ala
                   565             570
```

CLAIMS

1. A method of constructing a variant of a parent *Coprinus* laccase, which variant has laccase activity and improved 5 stability as compared to said parent laccase, which method comprises

i) analysing the structure of the parent *Coprinus* laccase to identify at least one amino acid residue or at least one 10 structural part of the *Coprinus* laccase structure, which amino acid residue or structural part is believed to be of relevance for altering the stability of the parent *Coprinus* laccase (as evaluated on the basis of structural or functional considerations),
15
ii) constructing a *Coprinus* laccase variant, which as compared to the parent *Coprinus* laccase, has been modified in the amino acid residue or structural part identified in i) so as to alter the stability, and, optionally,
20
iii) testing the resulting *Coprinus* laccase variant with respect to stability.

2. The method according to claim 1, wherein the structural part 25 to be modified is at the type I Cu site or at the type III Cu site.

3. A variant of a parent *Coprinus* laccase, which comprises a mutation in a position corresponding to at least one of the 30 following positions in SEQ ID No. 1:
W125,
Y134,
Y126,
Y170,
35 M75, and/or
M477.
4. A method of constructing a variant of a parent *Coprinus*-like

laccase, which variant has laccase activity and improved stability as compared to said parent laccase, which method comprises

i) comparing the three-dimensional structure of the *Coprinus*
5 laccase with the structure of a *Coprinus*-like laccase,

ii) identifying a part of the *Coprinus*-like laccase structure which is different from the *Coprinus* laccase structure and which from structural or functional considerations is contemplated to be responsible for differences in the stability
10 of the *Coprinus* and *Coprinus*-like laccase,

iii) modifying the part of the *Coprinus*-like laccase identified in ii) whereby a *Coprinus*-like laccase variant is obtained, which has an improved stability compared to the parent *Coprinus*-like laccase, and optionally,
15 iv) testing the resulting *Coprinus*-like laccase variant with respect to stability.

5. The method according to claim 4, wherein, in step iii), the part of the *Coprinus*-like laccase is modified so as to resemble
20 the corresponding part of the *Coprinus* laccase.

6. The method according to claim 4 or 5, wherein, in step iii), the modification is accomplished by deleting one or more amino acid residues of the part of the *Coprinus*-like laccase to be
25 modified; or the modification is accomplished by replacing one or more amino acid residues of the part of the *Coprinus*-like laccase to be modified with the amino acid residues occupying corresponding positions in the *Coprinus* laccase; or the modification is accomplished by insertion of one or more amino
30 acid residues present in the *Coprinus* laccase into a corresponding position in the *Coprinus*-like laccase.

7. The method according to any of claims 4-6, wherein the *Coprinus*-like laccase is selected from the group consisting of
35 *Polyporus pinsitus* laccase, *Phlebia radiata* laccase, *Rhizoctonia solani* laccase, *Scytalidium thermophilum* laccase

and *Myceliophthora thermophila* laccase.

8. The method according to claim 1 or 4, wherein the parent *Coprinus* laccase is derived from a strain of *Coprinus cinereus*.

9. The method according to claim 8, wherein the parent *Coprinus* laccase is derived from *Coprinus cinereus* IFO 8371.

10. A variant of a parent *Polyporus pinsitus (I)* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 2:
W107,
Y116,
Y108,
Y152,
M57, and/or
M328.

11. A variant of a parent *Polyporus pinsitus (II)* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 3:
W107,
Y116,
Y108,
Y152, and/or
M57.

12. A variant of a parent *Phlebia radiata* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 4:
W128,
Y137,
Y129,
Y137, and/or
M78.

13. A variant of a parent *Rhizoctonia solani (I)* laccase, which

comprises a mutation in a position corresponding to at least
one of the following positions in SEQ ID No. 5:
W126,
Y135,
5 Y127,
Y171, and/or
M76.

14. A variant of a parent *Rhizoctonia solani (II)* laccase,
10 which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 6:
W439,
W125,
Y134,
15 Y126,
Y170, and/or
M75.

15. A variant of a parent *Rhizoctonia solani (III)* laccase,
20 which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 7:
W411,
W125,
Y134,
25 Y126,
Y170, and/or
M75.

16. A variant of a parent *Rhizoctonia solani (IV)* laccase,
30 which comprises a mutation in a position corresponding to at
least one of the following positions in SEQ ID No. 8:
W411,
W125,
Y134,
35 Y126,
Y170, and/or
M75.

17. A variant of a parent *Scytalidium thermophilum* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 9:

5 M483,

W422,

W181,

Y190,

M530,

10 Y182,

Y221,

M300, and/or

M313.

15 18. A variant of a parent *Myceliophthora thermophila* laccase, which comprises a mutation in a position corresponding to at least one of the following positions in SEQ ID No. 10:

W507,

M433,

20 W373,

W136,

Y145,

M480,

Y137,

25 Y176, and/or

M254.

19. A DNA construct comprising a DNA sequence encoding a laccase variant according to claim 3 or claims 10-18.

30

20. A recombinant expression vector which carries a DNA construct according to claim 19.

21. A cell which is transformed with a DNA construct according 35 to claim 19 or a vector according to claim 20.

22. A cell according to claim 21, which is a microorganism.

23. A cell according to claim 22, which is a bacterium or a fungus.

5 24. A cell according to claim 23, which is an *Aspergillus niger* or an *Aspergillus oryzae* cell.

25. Use of a laccase variant according to claim 3 or claims 10-18 for oxidizing a substrate.

10

26. Use of a laccase variant according to claim 25 for dye transfer inhibition.

27. Use of a laccase variant according to claim 25 for 15 bleaching textiles, in particular for bleaching denim.

28. A detergent additive comprising a laccase variant according to claim 3 or claims 10-18 in the form of a non-dusting granulate, a stabilised liquid or a protected enzyme.

20

29. A detergent additive according to claim 28, which additionally comprises one or more other enzyme such as a protease, a lipase, an amylase, and/or a cellulase.

25 30. A detergent composition comprising a laccase variant according to claim 3 or claims 10-18 and a surfactant.

31. A detergent composition according to claim 30 which additionally comprises one or more other enzymes such as a 30 protease, a lipase, an amylase and/or a cellulase.

INTERNATIONAL SEARCH REPORT

A. CLASSIFICATION OF SUBJECT MATTER

IPC6: C12N 9/02 // (C12N 9/02, C12R 1:645)

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC6: C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

SE,DK,FI,NO classes as above

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used).

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 9606930 A1 (NOVO NORDISK A/S), 7 March 1996 (07.03.96)	1-31
	--	
X	WO 9600290 A1 (NOVO NORDISK BIOTECH, INC.), 4 January 1996 (04.01.96)	3,10-31
	--	
X	WO 9507988 A1 (NOVO NORDISK A/S), 23 March 1995 (23.03.95)	3,10-31
	--	
X	WO 9533837 A1 (NOVO NORDISK BIOTECH, INC.), 14 December 1995 (14.12.95)	3,10-31
	--	

[X] Further documents are listed in the continuation of Box C.   [X] See patent family annex.

*	Special categories of cited documents:	"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	
"E"	erlier document but published on or after the international filing date	"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"O"	document referring to an oral disclosure, use, exhibition or other means	
"P"	document published prior to the international filing date but later than the priority date claimed	"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
31 March 1998	0 1 -04- 1998
Name and mailing address of the ISA/	Authorized officer
Swedish Patent Office Box 5055, S-102 42 STOCKHOLM Facsimile No. +46 8 666 02 86	Patrick Andersson Telephone No. +46 8 782 25 00

Form PCT/ISA/210 (second sheet) (July 1992)

INTERNATIONAL SEARCH REPORT

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 9533836 A1 (NOVO NORDISK BIOTECH, INC.), 14 December 1995 (14.12.95) --	3,10-31
A	WO 9623874 A1 (NOVO NORDISK A/S), 8 August 1996 (08.08.96), see claims and the whole document --	1-2,4-9
A	Biochimica et Biophysica Acta, Volume 1292, 1996, Feng Xu et al, "A study of a series of recombinant fungal leaccases and bilirubin oxidase that exhibit significant differences in redox potential, substrate specificity, and stability", page 303 - page 311, page 310 --	1-2,4-9
A	FEMS Microbiology Letters, Volume 132, 1995, Soon-ja Kim et al, "Characteristics of a laccase over-secreting mutant of Coprinus congregatus" page 177 - page 179 -- --------	1-18

Patent document cited in search report			Publication date	Patent family member(s)			Publication date
WO	9606930	A1	07/03/96	AU	3253695	A	22/03/96
WO	9600290	A1	04/01/96	AU	2827895	A	19/01/96
				CA	2193070	A	04/01/96
				EP	0767836	A	16/04/97
				FI	965201	A	21/02/97
				US	5667531	A	16/09/97
WO	9507988	A1	23/03/95	AU	7833694	A	03/04/95
				BR	9407511	A	07/01/97
				CA	2171288	A	23/03/95
				CN	1133067	A	09/10/96
				EP	0719337	A	03/07/96
				FI	961250	A	18/03/96
				JP	9503126	T	31/03/97
				US	5480801	A	02/01/96
WO	9533837	A1	14/12/95	AU	2656695	A	04/01/96
				EP	0763115	A	19/03/97
WO	9533836	A1	14/12/95	AU	2656595	A	04/01/96
				CA	2191718	A	14/12/95
				EP	0765394	A	02/04/97
				FI	964808	A	02/12/96
WO	9623874	A1	08/08/96	AU	4483496	A	21/08/96
				CA	2211316	A	08/08/96
				EP	0808363	A	26/11/97

Form PCT/ISA/210 (patent family annex) (July 1992)

THIS PAGE BLANK (USPTO)